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SINCE FILE TOTAL ENTRY SESSION 0.22 0.22

FULL ESTIMATED COST

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http://www.cas.org/support/stngen/stndoc/properties.html

= >

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chain nodes :

12 14 15 16 17 18

ring nodes :

1 2 3 4 5 6 7 8 9 10

chain bonds :

1-14 7-12 14-15 15-16 16-17 17-18

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10

exact/norm bonds :

 $1 - 14 \quad 5 - 7 \quad 6 - 10 \quad 7 - 8 \quad 7 - 12 \quad 8 - 9 \quad 9 - 10 \quad 14 - 15 \quad 16 - 17 \quad 17 - 18$

exact bonds :

15-16

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1:0, N, Ak

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR

G1 O, N, Ak

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 16:40:01 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1131 TO ITERATE

100.0% PROCESSED 1131 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 20603 TO 24637 PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 16:40:05 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 22768 TO ITERATE

100.0% PROCESSED 22768 ITERATIONS SEARCH TIME: 00.00.01

ITERATIONS 0 ANSWERS

L3 0 SEA SSS FUL L1

=> fil stnguide COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 186.36 186.58

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FILE CONTAINS CURRENT INFORMATION.
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=> fil reg

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.14 186.72

FULL ESTIMATED COST

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http://www.cas.org/support/stngen/stndoc/properties.html

=>

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φ^{*}

chain nodes :
12 14 15
ring nodes :

1 2 3 4 5 6 7 8 9 10

chain bonds : 1-14 7-12 14-15 ring bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 5-7 \quad 6-10 \quad 7-8 \quad 8-9 \quad 9-10$

exact/norm bonds :

1-14 5-7 6-10 7-8 7-12 8-9 9-10 14-15 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 isolated ring systems : containing 1 :

G1:0, N, Ak

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:CLASS 14:CLASS 15:CLASS

L4STRUCTURE UPLOADED

=> d 14

L4 HAS NO ANSWERS L4STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s 14

SAMPLE SEARCH INITIATED 16:42:23 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 8456 TO ITERATE

23.7% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE** BATCH **COMPLETE**

163608 TO 174632 PROJECTED ITERATIONS: PROJECTED ANSWERS: 0 TO

0 SEA SSS SAM L4

=> s 14 sss full

FULL SEARCH INITIATED 16:42:27 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 168941 TO ITERATE

100.0% PROCESSED 168941 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.02

L6 1 SEA SSS FUL L4

=> d scan

REGISTRY COPYRIGHT 2009 ACS on STN 1 ANSWERS

2H-1, 4-Benzoxazine-6-butanoic acid,

3,4-dihydro-4-methyl- α , γ -dioxo-8-(phenylmethyl)-

C20 H19 N O5

ALL ANSWERS HAVE BEEN SCANNED

=> fil stnguide
COST IN U.S. DOLLARS

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION TULL ESTIMATED COST 186.36 373.08

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FILE CONTAINS CURRENT INFORMATION.
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=> fil reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION
0.21 373.29

FULL ESTIMATED COST

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TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>

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1 ANSWERS

chain nodes : 12 14 ring nodes : chain bonds : 1-14 7-12 14-18 ring bonds : $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 5-7 \quad 6-10 \quad 7-8 \quad 8-9 \quad 9-10 \quad 15-16 \quad 15-20 \quad 16-17 \quad 17-18$ 18-19 19-20 exact/norm bonds : 1-14 5-7 6-10 7-8 7-12 8-9 9-10 14-18 normalized bonds : $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 15-16 \quad 15-20 \quad 16-17 \quad 17-18 \quad 18-19 \quad 19-20$ isolated ring systems : containing 1 : 15 :

G1:0, N, Ak

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L7 STRUCTURE UPLOADED

=> d 17

L7 HAS NO ANSWERS

L7 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s 17

SAMPLE SEARCH INITIATED 16:44:51 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 8456 TO ITERATE

23.7% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 163608 TO 174632 PROJECTED ANSWERS: 1 TO 207

Г8 1 SEA SSS SAM L7 => s 17 sss full FULL SEARCH INITIATED 16:44:56 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 168941 TO ITERATE

100.0% PROCESSED 168941 ITERATIONS

78 ANSWERS

SEARCH TIME: 00.00.02

L9 78 SEA SSS FUL L7

=> d scan

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-8-[(1E)-2-[4-[4-(3-chlorophenoxy)butoxy]phenyl]ethenyl]-2,3dihydro-

MF C31 H32 C1 N O7

Double bond geometry as shown.

PAGE 1-A

PAGE 2-A

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):40

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN INDEX NAME NOT YET ASSIGNED

MF C32 H33 N O6

Double bond geometry as shown.

$$\begin{array}{c} \text{CO}_2\text{H} \\ \text{(CH}_2)_3 \\ \text{CO}_2\text{H} \\ \text{CO}_2\text{H} \\ \text{(CH}_2)_4 \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-8-[(1E)-2-[4-[2-(2,3-dihydro-1H-inden-2-yl)ethoxy]phenyl]ethenyl]-2,3-dihydro-

MF C32 H33 N O6

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN L9

4H-1, 4-Benzoxazine-4-butanoic acid, 2,3-dihydro-2-[(hydroxyamino)iminomethyl]-8-[2-[4-(4-phenylbutoxy)phenyl]ethenyl]-, ethyl ester IN

MFC33 H39 N3 O5

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-butanoic acid,

2-carboxy-2,3-dihydro-8-[(1E)-2-[4-[3-(2-

methylphenoxy)propoxy]phenyl]ethenyl]-

MF C31 H33 N O7

Double bond geometry as shown.

PAGE 1-A

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-2,3-dihydro- γ -oxo-8-[(1E)-2-[4-(4-phenylbutoxy)phenyl]ethenyl]-MF C31 H31 N O7

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-2,3-dihydro-8-[(1E)-2-[4-[3-(3-

methylphenoxy)propoxy]phenyl]ethenyl]-

MF C31 H33 N O7

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

REGISTRY COPYRIGHT 2009 ACS on STN L9 78 ANSWERS

IN

 $\begin{array}{l} 4 \text{H-1, 4-Benzoxazine-4-butanoic acid,} \\ 2 - (\text{aminocarbonyl}) - 2, 3 - \text{dihydro-8-[(1E)-2-[4-(4-phenylbutoxy)phenyl]ethenyl]-} \end{array}$

MF C31 H34 N2 O5

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-8-[(1E)-2-[4-[4-(2-fluorophenoxy)butoxy]phenyl]ethenyl]-2,3dihydro-

MF C31 H32 F N O7

Double bond geometry as shown.

PAGE 1-A

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-butanoic acid,

2-carboxy-2,3-dihydro-8-[2-[4-[3-(3-methoxyphenoxy)propoxy]phenyl]ethyl]-

MF C31 H35 N O8

PAGE 1-A

PAGE 2-A

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-2,3-dihydro-8-[(1E)-2-[4-[4-(2-methylphenoxy)butoxy]phenyl]ethenyl]-

MF C32 H35 N O7

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

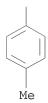
L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-butanoic acid,

2-carboxy-2,3-dihydro-8-[2-[4-[3-(4-methylphenoxy)propoxy]phenyl]ethyl]-

MF C31 H35 N O7

PAGE 2-A



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-2,3-dihydro-8-[(1E)-2-[4-[4-(3-methoxyphenoxy)butoxy]phenyl]ethenyl]-

MF C32 H35 N O8

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-butanoic acid,

2-carboxy-2,3-dihydro-8-[2-[4-[4-(2-methylphenoxy)butoxy]phenyl]ethyl]-

MF C32 H37 N O7

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-8-[(1E)-2-[4-[(2,3-dihydro-1H-inden-2-yl)oxy]phenyl]ethenyl]-2,3dihydro-

MF C30 H29 N O6

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-butanoic acid,

2-carboxy-2,3-dihydro-8-[2-[4-[4-(3-methoxyphenoxy)butoxy]phenyl]ethyl]-

MF C32 H37 N O8

PAGE 1-A

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-butanoic acid,

2-carboxy-2,3-dihydro-8-[(1E)-2-[4-(3-phenylpropoxy)phenyl]ethenyl]-

MF C30 H31 N O6

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1, 4-Benzoxazine-4-butanoic acid,

2-carboxy-2,3-dihydro-8-[2-[4-(3-phenylpropoxy)phenyl]ethyl]-

MF C30 H33 N O6

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-8-[(1E)-2-[4-[4-(2,6-dichlorophenoxy)butoxy]phenyl]ethenyl]-2,3dihydro-

MF C31 H31 C12 N O7

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-butanoic acid,

2-carboxy-2,3-dihydro-8-[(1E)-2-[4-(4-phenoxybutyl)phenyl]ethenyl]-

MF C31 H33 N O6

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-butanoic acid,

2-carboxy-2,3-dihydro-8-[(1E)-2-[4-(3-phenoxypropoxy)phenyl]ethenyl]-

MF C30 H31 N O7

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-butanoic acid,

 $2-(2,5-\text{dihydro}-5-\text{oxo}-1,2,4-\text{oxadiazol}-3-\text{yl})-2,3-\text{dihydro}-8-[(1\text{E})-2-[4-(4-\text{phenylbutoxy})\text{phenyl}]-\text{, ethyl ester}\\ \text{MF} \qquad \text{C34 H37 N3 O6}$

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-8-[(1E)-2-[4-[3-(4-fluorophenoxy)propoxy]phenyl]ethenyl]-2,3-dihydro-

MF C30 H30 F N O7

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-butanoic acid, 2-(ethoxycarbonyl)-2,3-dihydro-8-[(1E)-2-[4-(4-phenylbutoxy)phenyl]ethenyl]-

MF C33 H37 N O6

$$(CH_2)_{3}^{CO_2H}$$

$$N$$

$$OEt$$

$$(CH_2)_{4}^{O}$$

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-8-[(1E)-2-[4-[3-(3-fluorophenoxy)propoxy]phenyl]ethenyl]-2,3dihydro-

MF C30 H30 F N O7

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1, 4-Benzoxazine-4-butanoic acid, 2-(2,5-dihydro-5-oxo-1,2,4-thiadiazol-3-yl)-2,3-dihydro-8-[(1E)-2-[4-(4-phenylbutoxy)phenyl]ethenyl]-

MF C32 H33 N3 O5 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-butanoic acid,

2,3-dihydro-8-[2-[4-(4-phenylbutoxy)phenyl]ethyl]-2-(2H-tetrazol-5-yl)-

MF C31 H35 N5 O4

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-8-[(1E)-2-[4-[4-(4-fluorophenoxy)butoxy]phenyl]ethenyl]-2,3dihydro-

MF C31 H32 F N O7

Double bond geometry as shown.

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L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-butanoic acid,

2-carboxy-2,3-dihydro-8-[2-[4-[3-(2-methylphenoxy)propoxy]phenyl]ethyl]-

MF C31 H35 N O7

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PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

Double bond geometry as shown.

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PAGE 2-A

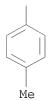
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-2,3-dihydro-8-[2-[4-[4-(4-methylphenoxy)butoxy]phenyl]ethyl]-

MF C32 H37 N O7

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-8-[(1E)-2-[4-[3-(2,3-dihydro-1H-inden-2-yl)propoxy]phenyl]ethenyl]-2,3-dihydro-

MF C33 H35 N O6

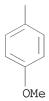
L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-butanoic acid,

2-carboxy-2,3-dihydro-8-[2-[4-[4-(4-methoxyphenoxy)butoxy]phenyl]ethyl]-

MF C32 H37 N O8

PAGE 1-A



L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1, 4-Benzoxazine-4-butanoic acid, 2-carboxy-8-[(1E)-2-[4-[(2,3-dihydro-1H-inden-2-yl)methoxy]phenyl]-2,3-dihydro-

MF C31 H31 N O6

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN 4H-1,4-Benzoxazine-4-butanoic acid,
 2-carboxy-8-[2-[4-[(2,3-dihydro-1H-inden-2-yl)methoxy]phenyl]ethyl]-2,3dihydro-
- MF C31 H33 N O6

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-butanoic acid, 2,3-dihydro-8-[(1E)-2-[4-(4-phenylbutoxy)phenyl]ethenyl]-2-[[(phenylsulfonyl)amino]carbonyl]-MF C37 H38 N2 O7 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN 4H-1,4-Benzoxazine-4-butanoic acid,
 2-carboxy-8-[(1E)-2-[4-[4-(2,6-dimethylphenoxy)butoxy]phenyl]ethenyl]-2,3dihydro-
- MF C33 H37 N O7

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PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 2H-1,4-Benzoxazine-6-butanoic acid,

N 2H-1,4-Benzoxazine-6-butanoic acid, 3,4-dihydro-4-methyl-α,γ-dioxo-8-(phenylmethyl)-

MF C20 H19 N O5

$$\begin{array}{c|c} O & O & Me \\ \parallel & \parallel & \parallel \\ HO_2C-C-CH_2-C & N \\ \hline \\ Ph-CH_2 & \end{array}$$

L9 78 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-8-[(1E)-2-[4-[3-(2-chlorophenoxy)propoxy]phenyl]ethenyl]-2,3dihydro-

MF C30 H30 C1 N O7

Double bond geometry as shown.

PAGE 1-A

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> fil cap
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 186.36 559.65

FULL ESTIMATED COST

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FILE 'REGISTRY' ENTERED AT 16:39:21 ON 03 FEB 2009

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 0 S L1 SSS FULL

FILE 'STNGUIDE' ENTERED AT 16:40:18 ON 03 FEB 2009

FILE 'REGISTRY' ENTERED AT 16:41:40 ON 03 FEB 2009

L4 STRUCTURE UPLOADED

L5 0 S L4

L6 1 S L4 SSS FULL

FILE 'STNGUIDE' ENTERED AT 16:42:44 ON 03 FEB 2009

FILE 'REGISTRY' ENTERED AT 16:44:34 ON 03 FEB 2009

L7 STRUCTURE UPLOADED

L8 1 S L7

L9 78 S L7 SSS FULL

FILE 'CAPLUS' ENTERED AT 16:45:30 ON 03 FEB 2009

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L10 2 L9

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L10 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:219785 CAPLUS

DOCUMENT NUMBER: 142:298120
TITLE: Preparation of

3,4-dihydro-2H-1,4-benzoxazine-2-carboxylic acid derivatives as cysLT2 receptor antagonists for

treatment of respiratory diseases

INVENTOR(S): Takeuchi, Jun; Itadani, Satoshi; Nakayama, Yoshisuke;

Tatsumi, Tadashi; Takahashi, Shinya; Fujita, Manabu

PATENT ASSIGNEE(S): Ono Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 237 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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	PATENT NO.)	DATE		APPLICATION NO.						DATE			
	WO 2005021518				A1	_	20050310		WO 2004-JP12563					20040831					
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	CA 2537355						CA 2004-2537355												
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	BR 2004013968				A					BR 2004-13968									
	MX 2006002152										MX 2006-2152								
							A 20061124				KR 2006-704215								
									NO 2006-1513 US 2006-569482										
	US 20060194797				A1		2006	0831								0060			
PRIOF	PRIORITY APPLN. INFO.:										2003-					0030			
												2003-					0031		
										,	WO	2004-	JP12	563	,	W 2	0040	831	

OTHER SOURCE(S): MARPAT 142:298120 GI

The title benzoxazine derivs. I [wherein R1 and R2 = independently (un)substituted acid group; D and E = independently a bond or a spacer; R3

bronchitis, pneumonia, severe acute respiratory syndrome (SARS), acute respiratory distress syndrome (ARDS), allergic rhinitis, sinusitis, etc. (no data). Formulations containing I as an active ingredient were also described. 847655-63-4P 847655-64-5P 847655-70-3P 847656-78-4P 847656-81-9P 847656-82-0P 847656-83-1P 847656-84-2P 847656-85-3P 847656-86-4P 847656-87-5P 847656-88-6P 847656-89-7P 847656-90-0P 847656-91-1P 847656-92-2P 847656-93-3P 847656-94-4P 847656-95-5P 847656-96-6P 847656-97-7P 847656-98-8P 847656-99-9P 847657-00-5P 847657-01-6P 847657-02-7P 847657-03-8P 847657-04-9P 847657-05-0P 847657-06-1P 847657-07-2P 847657-08-3P 847657-09-4P 847657-10-7P 847657-11-8P 847657-12-9P 847657-13-0P 847657-14-1P 847657-15-2P 847657-16-3P 847657-17-4P 847657-18-5P 847657-20-9P 847657-21-0P 847657-22-1P 847657-23-2P 847657-24-3P 847657-25-4P 847657-26-5P 847657-27-6P 847657-28-7P 847657-29-8P 847657-30-1P 847657-32-3P 847657-33-4P 847657-34-5P 847657-35-6P 847657-36-7P 847657-37-8P 847657-38-9P 847657-40-3P 847657-41-4P 847657-42-5P 847657-43-6P 847657-45-8P 847657-46-9P 847657-51-6P 847657-54-9P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (drug candidate; preparation of benzoxazine derivs. as cysLT2 receptor antagonists for treatment of respiratory diseases) RN 847655-63-4 CAPLUS CN 4H-1, 4-Benzoxazine-4-butanoic acid, 2-carboxy-2,3-dihydro-8-[(1E)-2-[4-(4-phenylbutoxy)phenyl]ethenyl]- (CA

= a substituent; ring A = (un)substituted cyclyl; ring B = (un)substituted cyclyl; Y and Z = independently C or N] or N-oxides, salts, solvates, or prodrugs thereof are prepared as cysteinyl leukotriene receptor LT-2 (cysLT2) antagonists. For example, the compound II was prepared in a multi-step synthesis. I inhibited cysLT2 with IC50 of <10 μ M. I are useful for the treatment of respiratory diseases, such as bronchial asthma, chronic obstructive lung disease, pulmonary emphysema, chronic

Double bond geometry as shown.

INDEX NAME)

RN 847655-64-5 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-2,3-dihydro-8-[2-[4-(4-phenylbutoxy)phenyl]ethyl]- (CA INDEX NAME)

RN 847655-70-3 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-2,3-dihydro-8-[(1Z)-2-[4-(4-phenylbutoxy)phenyl]ethenyl]- (CA INDEX NAME)

RN 847656-78-4 CAPLUS
CN 4H-1,4-Benzoxazine-4-butanoic acid,
2,3-dihydro-8-[(1E)-2-[4-(4-phenylbutoxy)phenyl]ethenyl]-2[[(phenylsulfonyl)amino]carbonyl]- (CA INDEX NAME)

Double bond geometry as shown.

RN 847656-81-9 CAPLUS
CN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-2,3-dihydro-8-[(1E)-2-[4-[(5-phenylpentyl)oxy]phenyl]ethenyl](CA INDEX NAME)

RN 847656-82-0 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-2,3-dihydro-8-[(1E)-2-[4-(4-phenoxybutoxy)phenyl]ethenyl]- (CA TNDEX NAME)

Double bond geometry as shown.

RN 847656-83-1 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-2,3-dihydro-8-[(1E)-2-[4-(3-phenylpropoxy)phenyl]ethenyl]- (CA INDEX NAME)

RN 847656-84-2 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-8-[(1E)-2-[4-[(2,3-dihydro-1H-inden-2-yl)methoxy]phenyl]ethenyl]-2,3-dihydro- (CA INDEX NAME)

Double bond geometry as shown.

RN 847656-85-3 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-8-[(1E)-2-[4-[(7-chloro-2-quinolinyl)methoxy]phenyl]ethenyl]-2,3-dihydro- (CA INDEX NAME)

RN 847656-86-4 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-8-[(1E)-2-[4-[[3-[(7-chloro-2-quinolinyl)methoxy]phenyl]methoxy]phenyl]ethenyl]-2,3-dihydro- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-B

RN 847656-87-5 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-8-[(1E)-2-[4-[(2,3-dihydro-1H-inden-2-yl)oxy]phenyl]ethenyl]-2,3-dihydro- (CA INDEX NAME)

Double bond geometry as shown.

RN 847656-88-6 CAPLUS
CN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-8-[(1E)-2-[4-[3-(2,3-dihydro-1H-inden-2-y1)propoxy]phenyl]ethenyl]-2,3-dihydro- (CA INDEX NAME)

Double bond geometry as shown.

RN 847656-89-7 CAPLUS
CN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-2,3-dihydro-8-[(1E)-2-[4-[4-(phenylmethoxy)butoxy]phenyl]ethenyl]- (CA INDEX NAME)

RN 847656-90-0 CAPLUS
CN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-2,3-dihydro-8-[(1E)-2-[4-[(5-phenoxypentyl)oxy]phenyl]ethenyl](CA INDEX NAME)

Double bond geometry as shown.

RN 847656-91-1 CAPLUS
CN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-2,3-dihydro-8-[(1E)-2-[4-[4-(3-methoxyphenoxy)butoxy]phenyl]ethenyl]- (CA INDEX NAME)

RN 847656-92-2 CAPLUS CN 4H-1,4-Benzoxazine-4-but

4H-1, 4-Benzoxazine-4-butanoic acid,

2-carboxy-2,3-dihydro-8-[(1E)-2-[4-[4-(4-

methoxyphenoxy)butoxy]phenyl]ethenyl]- (CA INDEX NAME)

RN 847656-93-3 CAPLUS
CN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-2,3-dihydro-8-[(1E)-2-[4-[4-(3-methylphenoxy)butoxy]phenyl]ethenyl]- (CA INDEX NAME)

RN 847656-94-4 CAPLUS
CN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-8-[(1E)-2-[4-[4-(3-fluorophenoxy)butoxy]phenyl]ethenyl]-2,3-dihydro- (CA INDEX NAME)

RN 847656-95-5 CAPLUS
CN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-2,3-dihydro-8-[(1E)-2-[4-[4-(2-methylphenoxy)butoxy]phenyl]ethenyl]- (CA INDEX NAME)

RN 847656-96-6 CAPLUS
CN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-8-[(1E)-2-[4-[4-(4-fluorophenoxy)butoxy]phenyl]ethenyl]-2,3-dihydro- (CA INDEX NAME)

RN 847656-97-7 CAPLUS
CN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-2,3-dihydro-8-[(1E)-2-[4-[4-(4-methylphenoxy)butoxy]phenyl]ethenyl]- (CA INDEX NAME)

Me

RN 847656-98-8 CAPLUS
CN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-2,3-dihydro-8-[(1E)-2-[4-[4-(2-methoxyphenoxy)butoxy]phenyl]ethenyl]- (CA INDEX NAME)

RN 847656-99-9 CAPLUS

CN

4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-8-[(1E)-2-[4-[4-(2-fluorophenoxy)butoxy]phenyl]ethenyl]-2,3-dihydro- (CA INDEX NAME)

Double bond geometry as shown.

RN

CN

RN 847657-01-6 CAPLUS
CN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-8-[(1E)-2-[4-[3-(4-chlorophenyl)propoxy]phenyl]ethenyl]-2,3-dihydro- (CA INDEX NAME)

RN 847657-02-7 CAPLUS CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-2,3-dihydro-8-[(1E)-2-[4-[3-(4-

methoxyphenyl)propoxy]phenyl]ethenyl]- (CA INDEX NAME)

RN 847657-03-8 CAPLUS
CN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-2,3-dihydro-8-[(1E)-2-[4-[3-(3-methylphenoxy)propoxy]phenyl]ethenyl]- (CA INDEX NAME)

RN 847657-04-9 CAPLUS
CN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-8-[(1E)-2-[4-[3-(3-fluorophenoxy)propoxy]phenyl]ethenyl]-2,3dihydro- (CA INDEX NAME)

RN 847657-05-0 CAPLUS
CN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-2,3-dihydro-8-[(1E)-2-[4-[3-(3-methoxyphenoxy)propoxy]phenyl]ethenyl]- (CA INDEX NAME)

RN 847657-06-1 CAPLUS
CN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-2,3-dihydro-8-[(1E)-2-[4-[3-(4-methylphenoxy)propoxy]phenyl]ethenyl]- (CA INDEX NAME)

847657-07-2 CAPLUS 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-2,3-dihydro-8-[(1E)-2-[4-[3-(2-methylphenoxy)propoxy]phenyl]ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.

RN

CN

RN 847657-08-3 CAPLUS

CN

4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-8-[(1E)-2-[4-[3-(4-fluorophenoxy)propoxy]phenyl]ethenyl]-2,3-dihydro- (CA INDEX NAME)

RN 847657-09-4 CAPLUS
CN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-2,3-dihydro-8-[(1E)-2-[4-[3-(4-methoxyphenoxy)propoxy]phenyl]ethenyl]- (CA INDEX NAME)

RN 847657-10-7 CAPLUS

CN

4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-8-[(1E)-2-[4-[3-(3-chlorophenoxy)propoxy]phenyl]ethenyl]-2,3-dihydro- (CA INDEX NAME)

RN 847657-11-8 CAPLUS
CN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-8-[(1E)-2-[4-[2-(2,3-dihydro-1H-inden-2-yl)ethoxy]phenyl]ethenyl]-2,3-dihydro- (CA INDEX NAME)

RN 847657-12-9 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-2,3-dihydro-8-[(1E)-2-[4-(3-phenoxypropoxy)phenyl]ethenyl]- (CA INDEX NAME)

RN 847657-13-0 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-8-[(1E)-2-[4-[3-(2-chlorophenoxy)propoxy]phenyl]ethenyl]-2,3-dihydro- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

RN 847657-14-1 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-8-[(1E)-2-[4-[4-(2-chlorophenoxy)butoxy]phenyl]ethenyl]-2,3-dihydro- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

PAGE 2-A

RN 847657-15-2 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-8-[(1E)-2-[4-[4-(3-chlorophenoxy)butoxy]phenyl]ethenyl]-2,3-dihydro- (CA INDEX NAME)

RN 847657-16-3 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-8-[(1E)-2-[4-[4-(2,6-dichlorophenoxy)butoxy]phenyl]ethenyl]-2,3-dihydro- (CA INDEX NAME)

RN 847657-17-4 CAPLUS

CN

4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-8-[(1E)-2-[4-[4-(2,6-dimethylphenoxy)butoxy]phenyl]ethenyl]-2,3-dihydro- (CA INDEX NAME)

Double bond geometry as shown.

RN 847657-18-5 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-8-[(1E)-2-[4-[4-(2-chloro-6-methylphenoxy)butoxy]phenyl]ethenyl]-2,3-dihydro- (CA INDEX NAME)

Double bond geometry as shown.

RN 847657-20-9 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-2,3-dihydro-8-[2-[4-(4-phenoxybutoxy)phenyl]ethyl]- (CA INDEX NAME)

RN 847657-21-0 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-2,3-dihydro-8-[2-[4-(3-phenylpropoxy)phenyl]ethyl]- (CA INDEX NAME)

RN 847657-22-1 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-8-[2-[4-[(2,3-dihydro-1H-inden-2-yl)methoxy]phenyl]ethyl]-2,3-dihydro- (CA INDEX NAME)

RN 847657-23-2 CAPLUS
CN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-8-[2-[4-[3-(2,3-dihydro-1H-inden-2-yl)propoxy]phenyl]ethyl]-2,3-dihydro- (CA INDEX NAME)

RN 847657-24-3 CAPLUS
CN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-2,3-dihydro-8-[2-[4-[(5-phenoxypentyl)oxy]phenyl]ethyl]- (CA
INDEX NAME)

RN 847657-25-4 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-2,3-dihydro-8-[2-[4-[4-(3-methoxyphenoxy)butoxy]phenyl]ethyl]-(CA INDEX NAME)

PAGE 1-A

RN 847657-26-5 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-2,3-dihydro-8-[2-[4-[4-(4-methoxyphenoxy)butoxy]phenyl]ethyl]-(CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 847657-27-6 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-2,3-dihydro-8-[2-[4-[4-(3-methylphenoxy)butoxy]phenyl]ethyl]-(CA INDEX NAME)

RN 847657-28-7 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid,

2-carboxy-8-[2-[4-[4-(3-fluorophenoxy)butoxy]phenyl]ethyl]-2,3-dihydro-(CA INDEX NAME)

RN 847657-29-8 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid,

2-carboxy-2,3-dihydro-8-[2-[4-[4-(2-methylphenoxy)butoxy]phenyl]ethyl]-(CA INDEX NAME)

RN 847657-30-1 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid,

2-carboxy-2,3-dihydro-8-[2-[4-[4-(4-methylphenoxy)butoxy]phenyl]ethyl]-(CA INDEX NAME)

RN 847657-32-3 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-2,3-dihydro-8-[2-[4-[4-(2-methoxyphenoxy)butoxy]phenyl]ethyl]-(CA INDEX NAME)

RN 847657-33-4 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid,

2-carboxy-8-[2-[4-[4-(2-fluorophenoxy)butoxy]phenyl]ethyl]-2,3-dihydro-(CA INDEX NAME)

RN 847657-34-5 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid,

2-carboxy-2,3-dihydro-8-[2-[4-[3-(4-methylphenoxy)propoxy]phenyl]ethyl]-(CA INDEX NAME)

RN 847657-35-6 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-2,3-dihydro-8-[2-[4-[3-(2-methylphenoxy)propoxy]phenyl]ethyl]-(CA INDEX NAME)

RN 847657-36-7 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid,

2-carboxy-2,3-dihydro-8-[2-[4-[3-(3-methylphenoxy)propoxy]phenyl]ethyl]-(CA INDEX NAME)

RN 847657-37-8 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-8-[2-[4-[3-(3-fluorophenoxy)propoxy]phenyl]ethyl]-2,3-dihydro-(CA INDEX NAME)

RN 847657-38-9 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid,

2-carboxy-2,3-dihydro-8-[2-[4-[3-(3-methoxyphenoxy)propoxy]phenyl]ethyl]-(CA INDEX NAME)

RN 847657-40-3 CAPLUS
CN 4H-1,4-Benzoxazine-4-butanoic acid,
2,3-dihydro-8-[2-[4-(4-phenylbutoxy)phenyl]ethyl]-2-(2H-tetrazol-5-yl)(CA INDEX NAME)

RN 847657-41-4 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2,3-dihydro-8-[(1E)-2-[4-(4-phenylbutoxy)phenyl]ethenyl]-2-(2H-tetrazol-5-yl)-, ethyl ester (CA INDEX NAME)

Double bond geometry as shown.

RN 847657-42-5 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2,3-dihydro-8-[(1E)-2-[4-(4-phenylbutoxy)phenyl]ethenyl]-2-(2H-tetrazol-5-yl)- (CA INDEX NAME)

Double bond geometry as shown.

RN 847657-43-6 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-(aminocarbonyl)-2,3-dihydro-8-[(1E)-2-[4-(4-phenylbutoxy)phenyl]ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.

RN 847657-45-8 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-(2,5-dihydro-5-oxo-1,2,4-thiadiazol-3-yl)-2,3-dihydro-8-[(1E)-2-[4-(4-phenylbutoxy)phenyl]ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.

RN 847657-46-9 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-(2,5-dihydro-5-oxo-1,2,4-oxadiazol-3-yl)-2,3-dihydro-8-[(1E)-2-[4-(4-phenylbutoxy)phenyl]ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.

RN 847657-51-6 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-(ethoxycarbonyl)-2,3-dihydro-8-[2-[4-(4-phenylbutoxy)phenyl]ethyl]- (CA INDEX NAME)

RN 847657-54-9 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-carboxy-2,3-dihydro- γ -oxo-8-[(1E)-2-[4-(4-phenylbutoxy)phenyl]ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.

IT 847657-81-2P 847657-82-3P 847657-83-4P
847657-86-7P 847657-87-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (intermediate; preparation of benzoxazine derivs. as cysLT2 receptor antagonists for treatment of respiratory diseases)
RN 847657-81-2 CAPLUS
CN 4H-1,4-Benzoxazine-4-butanoic acid,
2-(ethoxycarbonyl)-2,3-dihydro-8-[(1E)-2-[4-(4-phenylbutoxy)phenyl]ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.

RN 847657-82-3 CAPLUS
CN 4H-1,4-Benzoxazine-4-butanoic acid,
2-(ethoxycarbonyl)-2,3-dihydro-8-[(1E)-2-[4-(4-phenylbutoxy)phenyl]ethenyl]-, ethyl ester (CA INDEX NAME)

Double bond geometry as shown.

$$(CH_2)_3$$
 OET

N

OET

OCH2) 4

RN 847657-83-4 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-(ethoxycarbonyl)-2,3-dihydro-8-[2-[4-(4-phenylbutoxy)phenyl]ethyl]-, ethyl ester (CA INDEX NAME)

RN 847657-86-7 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2,3-dihydro-2-[(hydroxyamino)iminomethyl]-8-[2-[4-(4-phenylbutoxy)phenyl]ethenyl]-, ethyl ester (CA INDEX NAME)

RN 847657-87-8 CAPLUS

CN 4H-1,4-Benzoxazine-4-butanoic acid, 2-(2,5-dihydro-5-oxo-1,2,4-oxadiazol-3-yl)-2,3-dihydro-8-[(1E)-2-[4-(4-phenylbutoxy)phenyl]ethenyl]-, ethyl ester (CA INDEX NAME)

Double bond geometry as shown.

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1999:783939 CAPLUS

DOCUMENT NUMBER: 132:22755

TITLE: Preparation of aromatic and heteroaromatic

4-aryl-2,4-dioxobutyric acid derivatives useful as HIV

integrase inhibitors

INVENTOR(S): Young, Steven D.; Egbertson, Melissa; Payne, Linda S.;

Wai, John S.; Fisher, Thorsten E.; Guare, James P., Jr.; Embrey, Mark W.; Tran, Lee; Zhuang, Linghang; Vacca, Joseph P.; Langford, Marie; Melamed, Jeffrey;

Clark, David L.; Medina, Julio C.; Jaen, Juan

PATENT ASSIGNEE(S): Merck and Co., Inc., USA SOURCE: PCT Int. Appl., 319 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

P	PATENT NO.						KIND DATE				APPLICATION NO.					DATE		
W	WO 9962520				A1	A1 19991209			WO 1999-US12093					19990601				
		W:	ΑE,	AL,	AM,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	CA,	CN,	CU,	CZ,	EE,	GD,
			GE,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KG,	KR,	KZ,	LC,	LK,	LR,	LT,	LV,
			MD,	MG,	MK,	MN,	MX,	NO,	NΖ,	PL,	RO,	RU,	SG,	SI,	SK,	SL,	ТJ,	TM,
			TR,	TT,	UA,	US,	UZ,	VN,	YU,	ZA								
		RW:	GH,	GM,	ΚE,	LS,	MW,	SD,	SL,	SZ,	UG,	ZW,	ΑT,	BE,	CH,	CY,	DE,	DK,
			ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,
			CI,	CM,	GA,	GN,	GW,	ML,	MR,	NE,	SN,	TD,	TG					
C	CA 2333707				A1	19991209				CA 1999-2333707					19990601			
A	AU 9942254				Α	19991220			AU 1999-42254						19990601			
E)	P 1082121			A1	1 20010314			EP 1999-926094						19990601				
		R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙΤ,	LI,	LU,	NL,	SE,	PT,	IE,
			SI,	LT,	LV,	FI,	RO											
U	US 6380249					В1		2002	0430	US 1999-323417					19990601			
J1	JP 2002516863					T		2002	0611	JP 2000-551776					19990601			
PRIORI'	RIORITY APPLN. INFO.:									1	US 19	998-	8782	0P]	P 1	9980	603
									(GB 1	998-	1517.	5	Ž	A 1	9980	713	
										1	WO 1	999-1	US12	093	Ī	W 1	9990	601
	THE COURSE (C)							400		-								

OTHER SOURCE(S): MARPAT 132:22755

GΙ

Me
$$S$$
 CO_2H O O II

Certain six-membered aromatic and heteroarom. 2,4-dioxobutyric acid derivs. AB are described, specifically compds. ArCOCH2COCO2R [I; Ar = certain (un) substituted (hetero) aromatic groups; R = H, C1-6 alkyl]. I are inhibitors of HIV integrase, and are useful as inhibitors of HIV replication. The compds. are thus useful in the prevention or treatment of infection by HIV and the treatment of AIDS, either as compds., pharmaceutically acceptable salts, pharmaceutical composition ingredients, whether or not in combination with other antivirals [e.g., the HIV protease inhibitor indinavir], immunomodulators, antibiotics or vaccines. Methods of treating AIDS and methods of preventing or treating infection by HIV are also described. Over 200 specific compds. were prepared and/or claimed. For instance, title compound II was prepared as follows: (1) lithiation of 1,3-dibromobenzene and reaction with 5-methylthiophene-2-carboxaldehyde; (2) reduction of the resultant alc. with Et3SiH to give 2-(3-bromobenzyl)-5-methylthiophene; (3) lithiation of the latter bromide and acetylation with AcN(Me)OMe; (4) condensation of the

resultant Me ketone with di-Et oxalate; and (5) alkaline hydrolysis of the obtained Et ester. Representative compds. I inhibited HIV replication in T-lymphoid cells with IC95 values < 10 μM , and had IC50 values of < 1 μM in reference integrase and preintegration complex assays (no addnl. data).

IT 251964-24-6P, 4-(8-Benzyl-4-methyl-3,4-dihydro-2H-benzo[1,4]oxazin-6-yl)-2,4-dioxobutyric acid

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compound; preparation of aromatic and heteroarom. aryldioxobutyric

acid

derivs. as HIV integrase inhibitors)

RN 251964-24-6 CAPLUS

CN 2H-1,4-Benzoxazine-6-butanoic acid, 3,4-dihydro-4-methyl- α , γ -dioxo-8-(phenylmethyl)- (CA INDEX NAME)

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> fil stnguide COST IN U.S. DOLLARS SINCE FILE TOTAL. ENTRY SESSION FULL ESTIMATED COST 13.28 572.93 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE -1.64-1.64

FILE 'STNGUIDE' ENTERED AT 16:48:05 ON 03 FEB 2009 USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT COPYRIGHT (C) 2009 AMERICAN CHEMICAL SOCIETY (ACS)

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Jan 30, 2009 (20090130/UP).

=> fil req COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 0.42 573.35 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE 0.00 -1.64

FILE 'REGISTRY' ENTERED AT 16:51:57 ON 03 FEB 2009 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2009 American Chemical Society (ACS) Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 2 FEB 2009 HIGHEST RN 1099859-47-8 DICTIONARY FILE UPDATES: 2 FEB 2009 HIGHEST RN 1099859-47-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>

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chain nodes :

12 14

ring nodes :

1 2 3 4 5 6 7 8 9 10 15 16 17 18 19 20

chain bonds: 4-14 7-12 14-18 ring bonds:

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 15-16 15-20 16-17 17-18

18-19 19-20 exact/norm bonds:

4-14 5-7 6-10 7-8 7-12 8-9 9-10 14-18

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 15-16 15-20 16-17 17-18 18-19 19-20

isolated ring systems :
containing 1 : 15 :

G1:0, N, Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L11 STRUCTURE UPLOADED

=> d 111

L11 HAS NO ANSWERS

L11 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s 111

SAMPLE SEARCH INITIATED 16:53:11 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 8456 TO ITERATE

23.7% PROCESSED 2000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 163608 TO 174632
PROJECTED ANSWERS: 0 TO 0

L12 0 SEA SSS SAM L11

=> s l11 sss full

FULL SEARCH INITIATED 16:53:21 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 168941 TO ITERATE

100.0% PROCESSED 168941 ITERATIONS

4 ANSWERS

SEARCH TIME: 00.00.02

L13 4 SEA SSS FUL L11

=> d scan

L13 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2-Butenoic acid, 4-[(3R)-5-[(S)-(2,3-dimethoxyphenyl)hydroxymethyl]-3-(1,1-dimethylethyl)-2,3-dihydro-7-methyl-4H-1,4-benzoxazin-4-yl]-4-oxo-, ethyl ester, rel-

MF C28 H35 N O7

Relative stereochemistry.

Double bond geometry unknown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

L13 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-butanoic acid,

5-[(R)-(2,3-dimethoxyphenyl)hydroxymethyl]-3-(1,1-dimethylethyl)-2,3-

dihydro- β -mercapto-7-methyl- γ -oxo-, (3S)-rel-

MF C26 H33 N O7 S

Relative stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Ethanone, 2-bromo-1-[5-(2-fluorobenzoy1)-2,3-dihydro-4H-1,4-benzoxazin-4-y1]-

MF C17 H13 Br F N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Ethanone, 1-(5-benzoyl-2,3-dihydro-4H-1,4-benzoxazin-4-yl)-2-bromo-

MF C17 H14 Br N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=>

Uploading C:\Program Files\STNEXP\Queries\10569482other2.str

chain nodes :

12 14

ring nodes :

1 2 3 4 5 6 7 8 9 10 15 16 17 18 19 20

chain bonds :

3-14 7-12 14-18

ring bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 5-7 \quad 6-10 \quad 7-8 \quad 8-9 \quad 9-10 \quad 15-16 \quad 15-20 \quad 16-17 \quad 17-18$

18-19 19-20

exact/norm bonds :

3-14 5-7 6-10 7-8 7-12 8-9 9-10 14-18

normalized bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 15-16 \quad 15-20 \quad 16-17 \quad 17-18 \quad 18-19 \quad 19-20$

isolated ring systems :

containing 1 : 15 :

G1:0, N, Ak

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L14 STRUCTURE UPLOADED

=> s 114

SAMPLE SEARCH INITIATED 16:54:38 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 8456 TO ITERATE

23.7% PROCESSED 2000 ITERATIONS

1 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

41 ANSWERS

PROJECTED ITERATIONS: 163608 TO 174632 PROJECTED ANSWERS: 1 TO 207

L15 1 SEA SSS SAM L14

=> s 114 sss full

FULL SEARCH INITIATED 16:54:45 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 168941 TO ITERATE

100.0% PROCESSED 168941 ITERATIONS

SEARCH TIME: 00.00.02

L16 41 SEA SSS FUL L14

=> d scan

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN INDEX NAME NOT YET ASSIGNED

MF C25 H21 N O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):40

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN INDEX NAME NOT YET ASSIGNED

MF C26 H21 C1 F7 N O3

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 2H-1,4-Benzoxazin-3(4H)-one, 6-benzoyl-4-methyl-MF C16 H13 N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN INDEX NAME NOT YET ASSIGNED
MF C24 H18 F7 N O3

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 2H-1,4-Benzoxazin-3(4H)-one, 6-(4-chlorobenzoyl)-2,4-dimethyl-MF C17 H14 C1 N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 4H-1,4-Benzoxazine-4-carboxylic acid, 6-(ethylphenylamino)-2,3-dihydro-,
1,1-dimethylethyl ester
MF C21 H26 N2 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzenepropanoic acid, 4-[2-[2,3-dihydro-6-[(methoxyimino)phenylmethyl]-3-

 $oxo-4H-1, 4-benzoxazin-4-yl]ethoxy]-\alpha-ethoxy-$

MF C29 H30 N2 O7

$$\begin{array}{c|c} \text{OEt} \\ \text{HO}_2\text{C}-\text{CH}-\text{CH}_2 \\ \\ \text{O} \\ \text{CH}_2 \\ \\ \text{CH}_2 \\ \\ \text{CH}_2 \\ \\ \text{CH}_2 \\ \\ \text{O} \\ \\ \text{O} \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine, 6-(4-chloro-3-ethylphenoxy)-3,4-dihydro-4-[[3-(1,1,2,2,2-pentafluoroethyl)phenyl]methyl]-2-(trifluoromethyl)-, (2R)-

MF C26 H20 C1 F8 N O2

Absolute stereochemistry.

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzonitrile, 4-[(3,4-dihydro-4-methyl-3-oxo-2H-1,4-benzoxazin-6yl)hydroxymethyl]-

MF C17 H14 N2 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine, 3,4-dihydro-6-phenoxy-2-(trifluoromethyl)-4-[[3-(trifluoromethyl)phenyl]methyl]-, (2R)-

MF C23 H17 F6 N O2

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzonitrile, 4-[(3,4-dihydro-4-methyl-3-oxo-2H-1,4-benzoxazin-6-yl)-1Himidazol-1-ylmethyl]-

MF C20 H16 N4 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 2H-1,4-Benzoxazin-3(4H)-one, 6-(2-chloro-2-phenylacetyl)-4-methyl-MF C17 H14 Cl N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 2H-1,4-Benzoxazin-3(4H)-one, 6-(4-chlorobenzoyl)-4-methyl-MF C16 H12 C1 N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 8-methoxy-4-methyl-6-[phenyl(3S)-3-pyrrolidinylamino]MF C20 H23 N3 O3

Absolute stereochemistry.

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Methanone, [4-[2-(3,4-dimethoxyphenyl)ethyl]-3,4-dihydro-2H-1,4-benzoxazin-6-yl]phenyl-

MF C25 H25 N O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-carboxylic acid,

2,3-dihydro-5-methyl-3-oxo-6-(2-phenylethenyl)-, 1,1-dimethylethyl ester

MF C22 H23 N O4

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN INDEX NAME NOT YET ASSIGNED MF C28 H23 C1 F3 N O3

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzonitrile, 4-[(3,4-dihydro-4-methyl-3-oxo-2H-1,4-benzoxazin-6-yl)carbonyl]MF C17 H12 N2 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine, 6-(4-chloro-3-ethylphenoxy)-3,4-dihydro-2(trifluoromethyl)-4-[[3-[(trifluoromethyl)thio]phenyl]methyl]-, (2R)
MF C25 H20 C1 F6 N O2 S

Absolute stereochemistry.

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzoic acid, 2-[(3,4-dihydro-3-oxo-4-propyl-2H-1,4-benzoxazin-6yl)carbonyl]-

MF C19 H17 N O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 4-methyl-6-(2-phenylacetyl)-

MF C17 H15 N O3

$$\begin{array}{c|c} O & \text{Me} \\ \parallel & \parallel \\ \text{Ph-CH}_2-C & N & O \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzoic acid, 2-[[4-[(3-fluorophenyl)methyl]-3,4-dihydro-3-oxo-2H-1,4-benzoxazin-6-yl]carbonyl]-

MF C23 H16 F N O5

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzenepropanoic acid, $4-[2-[2,3-dihydro-6-[(methoxyimino)phenylmethyl]-3-oxo-4H-1,4-benzoxazin-4-yl]ethoxy]-<math>\alpha$ -ethoxy-, ethyl ester

MF C31 H34 N2 O7

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazin-3(4H)-one, 6-[2-chloro-4-(trifluoromethyl)phenoxy]-2, 4-dimethyl-

MF C17 H13 C1 F3 N O3

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzoic acid, 2-[[4-[2-(4-fluorophenyl)-2-oxoethyl]-3,4-dihydro-3-oxo-2H1,4-benzoxazin-6-yl]carbonyl]
MF C24 H16 F N O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine, 3,4-dihydro-4-[[3-(1,1,2,2,2pentafluoroethyl)phenyl]methyl]-6-phenoxy-2-(trifluoromethyl)-, (2R)
MF C24 H17 F8 N O2

Absolute stereochemistry.

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 4-methyl-6-(phenyl-1H-1,2,4-triazol-1ylmethyl)-

MF C18 H16 N4 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN INDEX NAME NOT YET ASSIGNED MF C26 H20 C1 F8 N O3

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazin-3(4H)-one, 6-benzoyl-2, 4-dimethyl-MF C17 H15 N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-6-amine, N-ethyl-3,4-dihydro-4-(1H-imidazol-5-ylmethyl)N-phenylMF C20 H22 N4 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzoic acid, 2-[(3,4-dihydro-4-methyl-3-oxo-2H-1,4-benzoxazin-6 yl)carbonyl]MF C17 H13 N O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzenepropanoic acid, $4-[2-[2,3-dihydro-6-[(hydroxyimino)phenylmethyl]-3-oxo-4H-1,4-benzoxazin-4-yl]ethoxy]-<math>\alpha$ -ethoxy-

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine, 6-(4-chloro-3-ethylphenoxy)-3,4-dihydro-2(trifluoromethyl)-4-[[3-(trifluoromethyl)phenyl]methyl]-, (2R)
MF C25 H20 C1 F6 N O2

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 2H-1,4-Benzoxazin-3(4H)-one, 6-(hydroxyphenylmethyl)-4-methyl-MF C16 H15 N O3

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN INDEX NAME NOT YET ASSIGNED MF C20 H18 N4 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 2H-1,4-Benzoxazin-3(4H)-one, 6-(1H-imidazol-1-ylphenylmethyl)-4-methyl-MF C19 H17 N3 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 6-(2-bromo-2-phenylacetyl)-4-methylMF C17 H14 Br N O3

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzoic acid, 2-[(3,4-dihydro-2,4-dimethyl-3-oxo-2H-1,4-benzoxazin-6-yl)carbonyl]MF C18 H15 N O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzenepropanoic acid, $4-[2-[2,3-dihydro-6-[(hydroxyimino)phenylmethyl]-3-oxo-4H-1,4-benzoxazin-4-yl]ethoxy]-<math>\alpha$ -ethoxy-, ethyl ester MF C30 H32 N2 O7

L16 41 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzenecarboximidamide, 3-[4-[5-[(2R,6S)-2,6-dimethyl-1-piperidinyl]pentyl]-3,4-dihydro-3-oxo-6-(phenylamino)-2H-1,4-benzoxazin-2-yl]-, rel
MF C33 H41 N5 O2

Relative stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

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à
                                                           å<sub>oå</sub>
chain nodes :
12 14
ring nodes :
1 2 3 4 5 6 7 8 9 10 15 16 17 18 19 20
chain bonds :
2-14 7-12 14-18
ring bonds :
1-2 1-6 2-3
               3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 15-16 15-20 16-17 17-18
 18-19 19-20
exact/norm bonds :
2-14 5-7 6-10 7-8 7-12 8-9 9-10 14-18
normalized bonds :
1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 15-16 \quad 15-20 \quad 16-17 \quad 17-18 \quad 18-19 \quad 19-20
isolated ring systems :
containing 1 : 15 :
```

G1:0, N, Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L17 STRUCTURE UPLOADED

=> s 117 sss full FULL SEARCH INITIATED 16:56:35 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 168941 TO ITERATE

100.0% PROCESSED 168941 ITERATIONS SEARCH TIME: 00.00.02

246 ANSWERS

L18 246 SEA SSS FUL L17

=> d scan

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-7-amine, 3,4-dihydro-4-methyl-N-phenyl-N-(3S)-3-pyrrolidinyl
MF C19 H23 N3 O

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):100

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 4H-1,4-Benzoxazine-4-butanoic acid,
2-carboxy-2,3-dihydro-7-[(1E)-2-[4-(2-phenylethoxy)phenyl]ethenyl]MF C29 H29 N O6

Double bond geometry as shown.

- L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN β -Alanine, N-[[7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-2H-1,4-benzoxazin-2-yl]carbonyl]-, ethyl ester, mixt. with butyl 2-[4-[[5-(trifluoromethyl)-2-pyridinyl]oxy]phenoxy]propanoate (9CI)
- MF C23 H21 Cl F4 N2 O6 . C19 H20 F3 N O4
- CI MXS

CM 1

CM 2

- L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN 2H-1, 4-Benzoxazin-3(4H)-one, 2-acetyl-7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-2, 4-dimethyl-
- MF C19 H14 Cl F4 N O4

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxamide, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-N-(phenylmethyl)
MF C25 H19 C1 F4 N2 O4

$$\begin{array}{c|c} & \text{Me} \\ & \text{N} & \text{O} \\ & \text{N} & \text{O} \\ & \text{Me} \\ & \text{C-NH-CH}_2\text{-Ph} \\ & \text{O} & \text{O} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxylic acid,
7-[2-chloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-,
phenylmethyl ester

MF C25 H19 C1 F3 N O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-2,4-dimethyl-, (S)- (9CI)
MF C17 H12 C1 F4 N O3

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[3-(4-chlorophenyl)-1-oxo-2-propenyl]-4-methyl-, (E)- (9CI)
MF C18 H14 Cl N O3

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN INDEX NAME NOT YET ASSIGNED MF C20 H18 N4 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 4-methyl-7-(1-oxo-2-phenyl-2-propen-1-yl)MF C18 H15 N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Methanone, [4-[2-(3,4-dimethoxyphenyl)ethyl]-3,4-dihydro-2H-1,4-benzoxazin-7-yl][4-[[2-(3,4-dimethoxyphenyl)ethyl]methylamino]-3-methoxyphenyl]
MF C37 H42 N2 O7

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-2,4-dimethyl-2-[1-[(2-propyn-1-yloxy)imino]ethyl]MF C22 H17 C1 F4 N2 O4

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Glycine, N-[[7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-2H-1,4-benzoxazin-2-yl]carbonyl]-

MF C20 H15 C1 F4 N2 O6

$$\begin{array}{c|c} & \text{Me} \\ & & \\$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazine-2-carboxamide, 7-[2-chloro-4-(trifluoromethyl)phenoxy]-N-ethyl-3, <math>4-dihydro-2, 4-dimethyl-3-oxo-

MF C20 H18 C1 F3 N2 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazine-2-carboxylic acid,

7-[2,6-dichloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-, ethyl ester

MF C20 H16 C12 F3 N O5

$$\begin{array}{c|c} & \text{Me} \\ \hline \\ \text{C1} & \text{N} & \text{O} \\ \hline \\ \text{Me} & \\ \hline \\ \text{C2} & \text{Me} \\ \hline \\ \text{C3} & \text{C} & \text{OEt} \\ \hline \\ \text{O} & \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-chloro-4-(trifluoromethyl)phenoxy]-2,4-dimethyl-2-phenyl-

MF C23 H17 C1 F3 N 03

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 4-butyl-7-(4-methoxybenzoyl)-

MF C20 H21 N O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Methanone, [7-(4-aminophenoxy)-2,3-dihydro-4H-1,4-benzoxazin-4-yl][4-[(1-butyl-4-piperidinyl)oxy]phenyl]-

MF C30 H35 N3 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1, 4-Benzoxazine-4-butanoic acid,

2-carboxy-2,3-dihydro-7-[(1E)-2-[4-(4-phenylbutoxy)phenyl]ethenyl]-

MF C31 H33 N O6

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Propanoic acid, 2-[4-[(6-chloro-2-benzoxazolyl)oxy]phenoxy]-, ethyl ester, mixt. with 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-N-ethyl-3,4-

dihydro-2,4-dimethyl-3-oxo-2H-1,4-benzoxazine-2-carboxamide (9CI)

MF $C20^{\circ}H17$ C1 F4 N2 O4 . C18 H16 C1 N O5

CI MXS

CM 1

$$\begin{array}{c|c} & \text{Me} \\ & & \text{N} \\ & & \text{O} \\ & & \text{Me} \\ & & \text{C-NHEt} \\ & & \text{O} \\ \end{array}$$

CM 2

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 2-(2-diazoacetyl)-7-[2,6-dichloro-4-(trifluoromethyl)phenoxy]-2,4-dimethyl-

MF C19 H12 C12 F3 N3 O4

$$\begin{array}{c|c} & & & & \\ & &$$

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxamide, 7-[2-chloro-6-fluoro-4-

(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-N-octyl-3-oxo-

MF C26 H29 C1 F4 N2 O4

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 2H-1,4-Benzoxazine-2-carboxylic acid,

7-[2-chloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-,4-chlorophenyl ester

MF C24 H16 C12 F3 N O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-2,4-dimethyl-, (R)- (9CI)
MF C17 H12 C1 F4 N O3

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN INDEX NAME NOT YET ASSIGNED MF C21 H22 N2 O3

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazin-3(4H)-one, 7-[3-(4-hydroxyphenyl)-1-oxo-2-propen-1-yl]-2,2,4-trimethyl-

MF C20 H19 N O4

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Methanone, [4-[2-(3,4-dimethoxyphenyl)]-3,4-dihydro-2H-1,4-benzoxazin-7-yl](4-methoxyphenyl)-

MF C26 H27 N O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-2,4-dimethyl-2-[1-[(2-propen-1-yloxy)imino]ethyl]-

MF C22 H19 C1 F4 N2 O4

$$\begin{array}{c|c} & \text{Me} \\ & \text{N} & \text{O} \\ & \text{N} & \text{O} \\ & \text{Me} \\ & \text{C-Me} \\ & \text{N-O-CH}_2\text{-CH} = \text{CH}_2 \\ \end{array}$$

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazine-2-carboxamide, 7-[2-chloro-4-(trifluoromethyl)phenoxy]-3, 4-dihydro-2, 4-dimethyl-3-oxo-

MF C18 H14 C1 F3 N2 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxylic acid,
7-[2-chloro-4-(trifluoromethyl)phenoxy]-2,4-diethyl-3,4-dihydro-3-oxo-,
ethyl ester

MF C22 H21 C1 F3 N O5

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazin-3(4H)-one, 7-[2-chloro-4-(trifluoromethyl)phenoxy]-2, 2, 4-trimethyl-

MF C18 H15 C1 F3 N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Ethanamine, 2-[[(3R,4S,5S)-5-[[3,4-dihydro-4-(3-methoxypropyl)-2H-1,4-benzoxazin-6-yl]methoxy]-4-[4-[(3,4-dihydro-4-methyl-2H-1,4-benzoxazin-7-yl)oxy]phenyl]-3-piperidinyl]oxy]-N-methyl-, relMF C36 H48 N4 O6

Relative stereochemistry.

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Methanone, [4-[(1-butyl-4-piperidinyl)oxy]phenyl][2,3-dihydro-7-(4-nitrophenoxy)-4H-1,4-benzoxazin-4-yl]-

MF C30 H33 N3 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-acetic acid, 7-benzoyl-2,3-dihydro- α ,3-dimethyl-2-oxo-, ethyl ester

MF C21 H21 N O5

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxamide, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-N-ethyl-3,4-dihydro-2,4-dimethyl-3-oxo-, mixt. with exo-1-methyl-4-(1-methylethyl)-2-[(2-methylphenyl)methoxy]-7-oxabicyclo[2.2.1]heptane (9CI)

MF C20 H17 C1 F4 N2 O4 . C18 H26 O2

CI MXS

CM 1

$$\begin{array}{c|c} & \text{Me} \\ & & \\$$

CM 2

Relative stereochemistry.

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-2-(2-diazoacetyl)-2,4-dimethyl-MF C19 H12 C1 F4 N3 O4

$$\begin{array}{c|c} F & Me \\ \hline N & O \\ \hline Me \\ \hline C-CH & N_2 \\ \hline O & O \\ \end{array}$$

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxamide, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-N-cyclohexyl-3,4-dihydro-2,4-dimethyl-3-oxo-

MF C24 H23 C1 F4 N2 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazine-2-carboxylic acid,

7-[2-chloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-,1,1-dimethylethyl ester

MF C22 H21 C1 F3 N 05

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazine, 7-[2-chloro-4-(trifluoromethyl)phenoxy]-3, 4-dihydro-2, 4-dimethyl-3-(nitromethylene)-

MF C18 H14 C1 F3 N2 O4

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazin-3(4H)-one, 2, 4-dimethyl-7-[(2E)-1-oxo-3-phenyl-2-propen-1-yl]-

MF C19 H17 N O3

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-7-butanoic acid,

3, 4-dihydro-4-[3-(1H-imidazol-2-ylamino)butyl]-3-oxo- β -phenyl-

MF C25 H28 N4 O4

$$\begin{array}{c|c} & & & \\ & & &$$

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazin-3(4H)-one, 7-[3-(4-chlorophenyl)-1-oxo-2-propen-1-yl]-1

2,2,4-trimethyl-C20 H18 Cl N O3

MF

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

7-y1](3,4,5-trimethoxyphenyl)-

MF C28 H31 N O7

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2,6-dichloro-4-(trifluoromethyl)phenoxy]-

2,4-dimethyl-2-[1-[(1-methylethoxy)imino]ethyl]-

MF C22 H21 C12 F3 N2 O4

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN β -Alanine, N-[[7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-2H-1,4-benzoxazin-2-yl]carbonyl]-, ethyl ester

MF C23 H21 C1 F4 N2 O6

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxylic acid,
 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl 3-oxo-, 2-(ethylamino)-2-oxoethyl ester
MF C22 H19 C1 F4 N2 O6

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxylic acid,
4-acetyl-7-[2-chloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2-methyl-3oxo-, ethyl ester

MF C21 H17 C1 F3 N O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazin-3(4H)-one, 7-[2-chloro-4-(trifluoromethyl)phenoxy]-4-methyl-

MF C16 H11 C1 F3 N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 3-Piperidinol, 5-[[3,4-dihydro-4-(3-methoxypropyl)-2H-1,4-benzoxazin-6yl]methoxy]-4-[4-[(3,4-dihydro-4-methyl-2H-1,4-benzoxazin-7-yl)oxy]phenyl], (3R,4R,5S)-rel-

MF C33 H41 N3 O6

Relative stereochemistry.

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Urea, N-[4-[4-[4-[4-[4-[4-[4-piperidiny]]]]-3,4-dihydro-2H-1,4-benzoxazin-7-yl]oxy]phenyl]-N'-(1-ethylpropyl)-

MF C36 H46 N4 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1, 4-Benzoxazine-4-acetic acid, 7-benzoyl-2, 3-dihydro-2-oxo-, ethylester

MF C19 H17 N O5

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Phosphoramidothioic acid, (1-methylpropyl)-, O-ethyl O-(5-methyl-2-nitrophenyl) ester, mixt. with 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-N-ethyl-3,4-dihydro-2,4-dimethyl-3-oxo-2H-1,4-benzoxazine-2-carboxamide (9CI)

MF C20 H17 C1 F4 N2 O4 . C13 H21 N2 O4 P S

CI MXS

CM 1

$$\begin{array}{c|c} & \text{Me} \\ & & \\$$

CM 2

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-2,4-dimethyl-2-(1-oxopentyl)-

MF C22 H20 C1 F4 N O4

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazine-2-carboxamide, N-butyl-7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-

MF C22 H21 C1 F4 N2 O4

$$\begin{array}{c|c} & & & \\ & & & \\$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazine-2-carboxylic acid,
7-[2-chloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-,
butyl ester
MF C22 H21 C1 F3 N O5

F3C N O Me O Me O C OBu-n

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 7-(3,5-dichlorophenoxy)-2,4-dimethylMF C16 H13 C12 N O3

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazin-3 (4H)-one, 4-methyl-7-(1-oxo-3-phenyl-2-propenyl)-, (E)-(9CI)

MF C18 H15 N O3

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2,4-Pentadienoic acid, 5-(3,4-dihydro-4-methyl-2H-1,4-benzoxazin-7-yl)-5-[4-(trifluoromethyl)phenyl]-, (2E,4Z)-

MF C21 H18 F3 N O3

Double bond geometry as shown.

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazin-3(4H)-one, 2,2,4-trimethyl-7-(1-oxo-3-phenyl-2-propen-1-yl)-

MF C20 H19 N O3

$$Ph-CH=CH-C \\ 0 \\ Me$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Ethanone, 1-[4-[2-(3,4-dimethoxyphenyl)ethyl]-3,4-dihydro-2H-1,4-benzoxazin-7-yl]-2-phenyl-

MF C26 H27 N O4

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-2-[1-(ethoxyimino)ethyl]-2,4-dimethyl-MF C21 H19 Cl F4 N2 O4

$$\begin{array}{c|c} & \text{Me} \\ & & \\$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Glycine, N-[[7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro2,4-dimethyl-3-oxo-2H-1,4-benzoxazin-2-yl]carbonyl]-, ethyl ester

MF C22 H19 C1 F4 N2 O6

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxylic acid,
7-[2-chloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-,
2-ethoxy-2-oxoethyl ester

MF C22 H19 C1 F3 N O7

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxylic acid,
7-[2-chloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-4-(methoxymethyl)-2methyl-3-oxo-, ethyl ester

MF C21 H19 C1 F3 N O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-chloro-4-(trifluoromethyl)phenoxy]-2methyl-4-(2-propyn-1-yl)-

MF C19 H13 C1 F3 N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetamide, $\alpha-[[(1S)-1-(3,4-dihydro-4-methyl-2H-1,4-benzoxazin-7-yl)-3-[4-(trifluoromethyl)phenyl]propyl]amino]-N-methyl-, (<math>\alpha$ R)-

MF C28 H30 F3 N3 O2

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 3-Piperidinol, 5-[[3,4-dihydro-4-(3-methoxypropyl)-2H-1,4-benzoxazin-6-yl]methoxy]-4-[4-[(3,4-dihydro-4-methyl-2H-1,4-benzoxazin-7-yl)oxy]phenyl]-1-[(4-methylphenyl)sulfonyl]-

MF C40 H47 N3 O8 S

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[(R)-1H-imidazol-1-ylphenylmethyl]-4-methylMF C19 H17 N3 O2

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 2H-1,4-Benzoxazine-2-carboxamide, 7-[2-chloro-6-fluoro-4-

(trifluoromethyl)phenoxy]-3,4-dihydro-N-(methoxymethyl)-2,4-dimethyl-3-oxo, mixt. with 2-chloro-N-(2,6-diethylphenyl)-N-(methoxymethyl)acetamide (9CI)

MF C20 H17 C1 F4 N2 O5 . C14 H20 C1 N O2

CI MXS

CM 1

CM 2

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-2,4-dimethyl-2-(1-oxobutyl)MF C21 H18 C1 F4 N O4

$$\begin{array}{c|c} & \text{Me} \\ & & \\$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazine-2-carboxamide, 7-[2-chloro-6-fluoro-4(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-N-(1-methylethyl)-3-oxoMF C21 H19 C1 F4 N2 O4

$$\begin{array}{c|c} & \text{Me} \\ & \text{N} & \text{O} \\ & \text{N} & \text{O} \\ & \text{Me} \\ & \text{C-NHPr-i} \\ & \text{O} \end{array}$$

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxylic acid,
7-[2-chloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-,
1-methylethyl ester

MF C21 H19 C1 F3 N O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine, 7-[2,6-dichloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-(nitromethylene)-

MF C18 H13 C12 F3 N2 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazin-3(4H)-one, 7-[3-(4-hydroxyphenyl)-1-oxo-2-propen-1-yl]-4-methyl-

MF C18 H15 N O4

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2,4-Pentadienamide, 5-(3,4-dihydro-4-methyl-2H-1,4-benzoxazin-7-yl)-N-5-isoquinolinyl-5-[4-(trifluoromethyl)phenyl]-, (2E,4Z)
MF C30 H24 F3 N3 O2

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[3-(4-hydroxyphenyl)-1-oxo-2-propen-1-yl]2,4-dimethyl
MF C19 H17 N O4

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Methanone, [4-[2-(3,4-dimethoxyphenyl)ethyl]-3,4-dihydro-2H-1,4-benzoxazin-7-yl]phenyl-

MF C25 H25 N O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazin-3(4H)-one, 7-[2,6-dichloro-4-(trifluoromethyl)phenoxy]-2-

[1-(methoxyimino)ethyl]-2,4-dimethyl-

MF C20 H17 C12 F3 N2 O4

$$\begin{array}{c|c} & \text{Me} & \\ & \text{N} & \text{O} \\ & \text{N} & \text{O} \\ & \text{N} & \text{OMe} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

MF C21 H17 C1 F4 N2 O6

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxylic acid, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-, 2,2,2-trifluoroethyl ester

MF C20 H13 C1 F7 N O5

$$\begin{array}{c|c} & \text{Me} & \\ & \text{N} & \text{O} \\ & \text{Me} \\ & \text{O} & \text{Me} \\ & \text{C1} & \text{C1} & \text{C} \\ & \text{O} \\ & \text{O} & \text{C} \\ & \text{O} \\ & \text{O} & \text{C} \\ & \text{O} \\ & \text{O}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxylic acid, 7-[2-chloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2-methyl-3-oxo-4-(phenylmethyl)-, ethyl ester

MF C26 H21 C1 F3 N O5

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-chloro-4-(trifluoromethyl)phenoxy]-2methyl-4-(1-methylethyl)-

MF C19 H17 C1 F3 N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetamide, $\alpha-[[(1R)-1-(3,4-\text{dihydro}-4-\text{methyl}-2H-1,4-\text{benzoxazin}-7-y1)-3-[4-(trifluoromethyl)phenyl]propyl]amino]-N-methyl-, (<math>\alpha$ S)-

MF C28 H30 F3 N3 O2

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzenesulfonamide, N-[2-[[5-[[3,4-dihydro-4-(3-methoxypropyl)-2H-1,4-benzoxazin-6-yl]methoxy]-4-[4-[(3,4-dihydro-4-methyl-2H-1,4-benzoxazin-7-yl)oxy]phenyl]-1-[(4-methylphenyl)sulfonyl]-3-piperidinyl]oxy]ethyl]-N,4-dimethyl-

MF C50 H60 N4 O10 S2

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[(S)-1H-imidazol-1-ylphenylmethyl]-4-methylMF C19 H17 N3 O2

Absolute stereochemistry.

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxamide, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-N-(methoxymethyl)-2,4-dimethyl-3-oxo-, mixt. with 2,6-dinitro-N,N-dipropyl-4-(trifluoromethyl)benzenamine (9CI)

MF C20 H17 C1 F4 N2 O5 . C13 H16 F3 N3 O4

CI MXS

CM 1

CM 2

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-2-(1-ethyl-1-hydroxypropyl)-2,4-dimethyl-MF C22 H22 Cl F4 N O4

$$\begin{array}{c|c} & \text{Me} \\ & & \\$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

$$\begin{array}{c|c} & \text{Me} \\ & \text{N} & \text{O} \\ & \text{N} & \text{O} \\ & \text{Me} \\ & \text{C-NHPr-n} \\ & \text{O} \end{array}$$

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxylic acid,
7-[2-chloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-,
propyl ester

MF C21 H19 C1 F3 N O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-(nitromethylene)-

MF C18 H13 C1 F4 N2 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 7-benzoyl-2,4-dimethyl-

MF C17 H15 N O3

$$\begin{array}{c|c} & Me & \\ & N & O \\ \hline & N & O \\ \hline & N & Me \\ \hline & O & Me \\ \hline & O & Me \\ \hline \end{array}$$

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-(4-hydroxyphenyl)acetyl]-2,2,4-trimethyl-MF C19 H19 N O4

$$\begin{array}{c|c} \text{Me} & \\ \\ \text{HO} & \\ \\ \text{CH}_2 - \\ \text{C} & \\ \\ \text{Me} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[3-(4-chlorophenyl)-1-oxo-2-propen-1-yl]2,4-dimethyl
MF C19 H16 C1 N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazine, 4-[2-(3,4-dimethoxyphenyl)ethyl]-3,4-dihydro-7-phenoxyMF C24 H25 N O4

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-chloro-6-fluoro-4(trifluoromethyl)phenoxy]-2-[1-(methoxyimino)ethyl]-2,4-dimethylMF C20 H17 C1 F4 N2 O4

$$\begin{array}{c|c} & \text{Me} & \\ & &$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxamide, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-N,N,2,4-tetramethyl-3-oxo-MF C20 H17 Cl F4 N2 O4

$$F_3C$$
 $C1$
 Me
 N
 O
 Me
 $C-NMe_2$

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazine-2-carboxylic acid,

7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-, 2-propyn-1-yl ester

MF C21 H14 C1 F4 N O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxylic acid,

7-[2-chloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2-methyl-3-oxo-4-(2-propen-1-yl)-, ethyl ester

MF C22 H19 C1 F3 N O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-chloro-4-(trifluoromethyl)phenoxy]-4-ethyl-2-methyl-

MF C18 H15 C1 F3 N O3

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):100

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

MF C19 H18 F3 N O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Ethanamine, 2-[[(3S,4R,5R)-5-[[3,4-dihydro-4-(3-methoxypropyl)-2H-1,4-benzoxazin-6-yl]methoxy]-4-[4-[(3,4-dihydro-4-methyl-2H-1,4-benzoxazin-7-yl)oxy]phenyl]-3-piperidinyl]oxy]-N-methyl-

MF C36 H48 N4 O6

Absolute stereochemistry.

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 7-(1H-imidazol-1-ylphenylmethyl)-4-methylMF C19 H17 N3 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazine-2-carboxamide, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-N-(2,2,2-trifluoroethyl)-, mixt. with exo-1-methyl-4-(1-methylethyl)-2-[(2-methylphenyl)methoxy]-7-oxabicyclo[2.2.1]heptane (9CI)
MF C20 H14 C1 F7 N2 O4 . C18 H26 O2

CI MXS

CM 1

$$\begin{array}{c|c} & \text{Me} \\ & \text{N} & \text{O} \\ & \text{N} & \text{O} \\ & \text{Me} \\ & \text{C-NH-CH}_2\text{-CF}_3 \\ & \text{O} \end{array}$$

CM 2

Relative stereochemistry.

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-2,4-dimethyl-2-(1-oxopropyl)MF C20 H16 C1 F4 N O4

$$\begin{array}{c|c} & \text{Me} \\ & & \\ \hline & & \\ & & \\ \hline & & \\ &$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazine-2-carboxamide, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-4-(difluoromethyl)-N-ethyl-3,4-dihydro-2-methyl-3-oxoMF C20 H15 C1 F6 N2 O4

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxylic acid,
7-[2-chloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-,
methyl ester

MF C19 H15 C1 F3 N O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Cyanamide, [7-[2-chloro-4-(trifluoromethyl)phenoxy]-2,4-dimethyl-2H-1,4benzoxazin-3(4H)-ylidene]- (9CI)

MF C18 H13 C1 F3 N3 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazin-3(4H)-one, 4-methyl-7-(1-oxo-3-phenyl-2-propen-1-yl)-1

MF C18 H15 N O3

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-(4-chlorophenyl)acetyl]-2,2,4-trimethylMF C19 H18 C1 N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 2,4-dimethyl-7-(1-oxo-3-phenyl-2-propen-1-yl)MF C19 H17 N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 2H-1,4-Benzoxazine-7-propanoic acid, 3,4-dihydro-4-[2-[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]acetyl]- β -(2-methylphenyl)-MF C35 H35 N3 O6

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-chloro-6-fluoro-4(trifluoromethyl)phenoxy]-2-[1-(hydroxyimino)ethyl]-2,4-dimethylMF C19 H15 C1 F4 N2 O4

$$\begin{array}{c|c} & \text{Me} \\ & \text{N} & \text{O} \\ & \text{N} & \text{O} \\ & \text{C1} & \text{Me} \\ & \text{N-OH} \end{array}$$

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazine-2-carboxamide, 7-[2-chloro-6-fluoro-4-

(trifluoromethyl)phenoxy]-3,4-dihydro-N-(methoxymethyl)-2,4-dimethyl-3-oxo-

MF C20 H17 C1 F4 N2 O5

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxylic acid,
7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl3-oxo-, 2-propen-1-yl ester

MF C21 H16 C1 F4 N O5

$$\begin{array}{c|c}
 & \text{Me} \\
 & \text{N} & \text{O} \\
 & \text{N} & \text{O} \\
 & \text{N} & \text{O} \\
 & \text{Me} \\
 & \text{C} & \text{O} & \text{CH}_2 & \text{CH} = \text{CH}_2 \\
 & \text{O} & \text{O} & \text{CH}_2 & \text{CH} = \text{CH}_2
\end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxylic acid,
7-[2-chloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2-methyl-4-(1methylethyl)-3-oxo-, ethyl ester

MF C22 H21 C1 F3 N O5

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-chloro-4-(trifluoromethyl)phenoxy]-2,4dimethyl-

MF C17 H13 C1 F3 N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetamide, $\alpha-[[(1R)-1-(3,4-dihydro-4-methyl-2H-1,4-benzoxazin-7-yl)-3-[4-(trifluoromethyl)phenyl]propyl]amino]-N-methyl-, <math>(\alpha R)$ -rel-

MF C28 H30 F3 N3 O2

Relative stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 3-Piperidinol, 5-[[3,4-dihydro-4-(3-methoxypropyl)-2H-1,4-benzoxazin-6-yl]methoxy]-4-[4-[(3,4-dihydro-4-methyl-2H-1,4-benzoxazin-7-yl)oxy]phenyl]-, (3S,4S,5R)
MF C33 H41 N3 O6

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 7-(hydroxyphenylmethyl)-4-methylMF C16 H15 N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Phosphoramidothioic acid, (1-methylpropyl)-, O-ethyl
O-(5-methyl-2-nitrophenyl) ester, mixt. with
7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl3-oxo-N-(2,2,2-trifluoroethyl)-2H-1,4-benzoxazine-2-carboxamide (9CI)

CI MXS

CM 1

$$\begin{array}{c|c} & \text{Me} \\ & \text{N} & \text{O} \\ & \text{Me} \\ & \text{C-NH-CH}_2\text{-CF}_3 \\ & \text{O} \end{array}$$

CM 2

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxylic acid, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-, 2,2-dimethylhydrazide

MF C20 H18 Cl F4 N3 O4

$$\begin{array}{c|c} & \text{Me} \\ & & \text{N} \\ & & \text{O} \\ & \text{Me} \\ & \text{O} \\ & \text{C} \\ & \text{NH- NMe}_2 \\ & \text{O} \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxamide, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-N-ethyl-3,4-dihydro-2,4-dimethyl-3-oxo-

MF C20 H17 C1 F4 N2 O4

CI COM

$$\begin{array}{c|c} & \text{Me} \\ & & \text{N} \\ & & \text{O} \\ & & \text{Me} \\ & & \text{C-NHEt} \\ & & \text{O} \\ \end{array}$$

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxylic acid,
7-[2-chloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-,
potassium salt (1:1)

MF C18 H13 C1 F3 N O5 . K

$$\begin{array}{c|c} & \text{Me} & \\ & &$$

K

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Propanedinitrile, 2-[7-[2-chloro-4-(trifluoromethyl)phenoxy]-2,4-dimethyl-2H-1,4-benzoxazin-3(4H)-ylidene]-

MF C20 H13 C1 F3 N3 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[3-(4-chlorophenyl)-1-oxo-2-propen-1-yl]-4-

methyl-MF C18 H14 C1 N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 2,2,4-trimethyl-7-(2-phenylacetyl)MF C19 H19 N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[5-chloro-2-[(methylamino)methyl]phenoxy]-4methylMF C17 H17 C1 N2 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Acetic acid, 2-(acetyloxy)-, 2-[7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-2H-1,4-benzoxazin-2-yl]-2-oxoethyl ester

MF C23 H18 C1 F4 N O8

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxamide, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-N-(2-methoxyethyl)-2,4-dimethyl-3-oxo-

MF C21 H19 C1 F4 N2 O5

CI COM

$$\begin{array}{c|c} & \text{Me} \\ & & \text{O} \\ & & \text{Me} \\ & & \text{O} \\ & & \text{C-NH-CH}_2\text{--CH}_2\text{--OMe} \\ & & \text{O} \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxylic acid,
 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl 3-oxo-, propyl ester
MF C21 H18 C1 F4 N O5

$$rac{F}{C1}$$
 $rac{Me}{N}$
 $rac{N}{N}$
 $rac{O}{N}$
 $rac{Me}{N}$
 $rac{N}{N}$
 $rac{O}{N}$
 $rac{Me}{N}$
 $rac{N}{N}$
 $rac{N}$
 $rac{N}{N}$
 $rac{N}$
 $rac{N}{N}$
 $rac{N}$
 $rac{N}$
 $rac{N}$
 $rac{N}$
 $rac{N}$
 $rac{N}$
 $rac{N}$
 $rac{N}$
 $rac{N}$

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxylic acid,

7-[2-chloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2-methyl-3-oxo-4-

propyl-, ethyl ester C22 H21 Cl F3 N O5

MF

F3C NO Me C-OEt

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazin-3 (4H)-one, 2, 4-dimethyl-7-(1-oxo-2-phenyl-2-propen-1-yl)-

MF C19 H17 N O3

$$\begin{array}{c|c} & \text{Me} \\ & & \\ & & \\ \text{N} & \text{O} \\ \\ \text{Ph-C-C} & \\ & & \\ \text{Me} \\ \\ \text{H}_2\text{C} & \text{O} \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetamide, α -[[(1R)-1-(3,4-dihydro-4-methyl-2H-1,4-benzoxazin-7-yl)-3-[4-(trifluoromethyl)phenyl]propyl]amino]-N-methyl-,

 (αS) -rel- MF C28 H30 F3 N3 O2

Relative stereochemistry.

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-(4-hydroxyphenyl)-1-oxo-2-propen-1-yl]2,2,4-trimethyl-

MF C20 H19 N O4

$$\begin{array}{c|c} & \text{Me} \\ & \text{N} \\ \hline \\ \text{C} \\ \text{CH}_2 \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzoic acid, 4-[[3,4-dihydro-4-methyl-3-oxo-7-(3-phenyl-1-propyn-1-yl)-2H-1,4-benzoxazin-2-yl]methyl]-

MF C26 H21 N O4

$$\begin{array}{c|c} & \text{Me} \\ & \\ & \\ \text{N} & \\ \text{O} & \\ \text{CH}_2 - \\ \text{C} & \\ \end{array} \\ \begin{array}{c} \text{CO}_2\text{H} \\ \\ \text{CH}_2 - \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Carbamothioic acid, diethyl-, S-[(4-chlorophenyl)methyl] ester, mixt. with 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl- <math>3-oxo-N-(2,2,2-trifluoroethyl)-2H-1,4-benzoxazine-2-carboxamide (9CI)

MF C20 H14 C1 F7 N2 O4 . C12 H16 C1 N O S

CI MXS

CM 1

CM 2

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Carbamothioic acid, [[7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-2H-1,4-benzoxazin-2-yl]carbonyl]-, O-ethyl ester (9CI)

MF C21 H17 C1 F4 N2 O5 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxamide, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-N,2,4-trimethyl-3-oxo-

MF C19 H15 C1 F4 N2 O4

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxylic acid,
7-[2-chloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-,
sodium salt (1:1)

MF C18 H13 C1 F3 N O5 . Na

Na

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazine-3(4H)-thione, 7-[2,6-dichloro-4-(trifluoromethyl)phenoxy]-2,4-dimethylMF C17 H12 C12 F3 N O2 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 2H-1,4-Benzoxazin-3(4H)-one, 7-(4-chlorobenzoyl)-2,2,4-trimethyl-MF C18 H16 Cl N O3

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazin-3(4H)-one, 7-[2-(4-hydroxyphenyl)acetyl]-2, 4-dimethyl-MF C18 H17 N O4

$$\begin{array}{c|c} & \text{Me} \\ & \\ \text{N} \\ \text{O} \\ \text{CH}_2 \\ \text{C} \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzenemethanamine, 4-chloro-2-[(3,4-dihydro-4-methyl-2H-1,4-benzoxazin-7-yl)oxy]-N-methyl-

MF C17 H19 C1 N2 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Phenol, 4-[[4-(dimethylamino)phenyl](4-ethyl-3,4-dihydro-2H-1,4-benzoxazin-7-yl)methyl]-2,6-dimethoxy-

MF C27 H32 N2 O4

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazin-3(4H)-one, 2-[2-(acetyloxy)acetyl]-7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-2, 4-dimethyl-

MF C21 H16 C1 F4 N O6

$$\begin{array}{c|c} & \text{Me} \\ & \text{N} & \text{O} \\ & \text{N} & \text{O} \\ & \text{Me} \\ & \text{C} & \text{CH}_2 - \text{OAc} \\ & \text{O} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazine-2-carboxamide, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-N-methoxy-2,4-dimethyl-3-oxo-MF C19 H15 C1 F4 N2 O5

$$\begin{array}{c|c} & & & \\ & & & \\$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazine-2-carboxylic acid,

7-[2,6-dichloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-,2-propen-1-yl ester

MF C21 H16 C12 F3 N O5

$$\begin{array}{c|c} & \text{Me} \\ & & \\ & & \\ \text{N} & \text{O} \\ & \text{Me} \\ & \text{C} & \text{O} & \text{CH}_2 - \text{CH} = \text{CH}_2 \\ & &$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxylic acid,

7-[2-chloro-4-(trifluoromethyl)phenoxy]-4-ethyl-3, 4-dihydro-2-methyl-3-oxo-2-m

, ethyl ester

MF C21 H19 C1 F3 N O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazin-3(4H)-one, 2, 4-dimethyl-7-(2-phenylacetyl)-

MF C18 H17 N O3

$$\begin{array}{c|c} & \text{Me} & \\ & & \\ N & \\ O & \\ \text{Ph-CH}_2-C & \\ & \\ O & \\ \end{array}$$

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazine-7-butanoic acid,

3,4-dihydro-3-oxo- β -phenyl-4-[3-(2-pyridinylamino)propyl]-, ethyl

ester

MF C28 H31 N3 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazin-3(4H)-one, 7-[2-(4-chlorophenyl)-1-oxo-2-propen-1-yl]-

2,2,4-trimethyl-

MF C20 H18 C1 N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazine-7-butanoic acid,

3, 4-dihydro-4-[4-(1H-imidazol-2-ylamino)butyl]-3-oxo- β -phenyl-

MF C25 H28 N4 O4

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN β -Alanine, N-[[7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-2H-1,4-benzoxazin-2-yl]carbonyl]-, ethyl ester, mixt. with 2-[1-(ethoxyimino)butyl]-5-[2-(ethylthio)propyl]-3-hydroxy-2-cyclohexen-1-one (9CI)

MF C23 H21 Cl F4 N2 O6 . C17 H29 N O3 S

CI MXS

CM 1

CM 2

$$\begin{array}{c} \text{SEt} \\ \text{Me-CH-CH}_2 \\ \text{OH} \\ \begin{array}{c} \text{C-Pr-n} \\ \text{N-OEt} \end{array}$$

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazine-2-carboxamide, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxoMF C18 H13 C1 F4 N2 O4

$$\begin{array}{c|c} & \text{Me} & \\ & &$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxylic acid,
7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl3-oxo
MF C18 H12 C1 F4 N O5

$$\begin{array}{c|c} & \text{Me} \\ \hline & \text{N} & \text{O} \\ \hline & \text{N} & \text{O} \\ \hline & \text{CO}_2 \text{H} \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazine-3(4H)-thione, 7-[2-chloro-6-fluoro-4-

(trifluoromethyl)phenoxy]-2,4-dimethyl-

MF C17 H12 C1 F4 N O2 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 7-(4-chlorobenzoy1)-2,4-dimethyl-

MF C17 H14 C1 N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

 $\label{eq:control_ent$

MF C18 H16 C1 N O3

$$\begin{array}{c|c} \text{C1} & \text{Me} \\ & \text{N} & \text{O} \\ \text{CH}_2 - \text{C} & \text{O} & \text{Me} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Methanone, (3,4-dihydro-4-methyl-2H-1,4-benzoxazin-7-yl)(3-ethoxy-4-

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2,5-Cyclohexadien-1-one, 4-[[4-amino-3,5-bis(1-methylethyl)phenyl](4-ethyl-3,4-dihydro-2H-1,4-benzoxazin-7-yl)methylene]-2,6-dimethoxy-

MF C31 H38 N2 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 2-(2-bromoacetyl)-7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-2,4-dimethyl-

MF C19 H13 Br Cl F4 N O4

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

MF C24 H16 Cl2 F4 N2 O4

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazine-2-carboxylic acid, 7-[2,6-dichloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-, 2-methoxyethyl ester

MF C21 H18 C12 F3 N O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxylic acid,
7-[2-chloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-,
ethyl ester

MF C20 H17 C1 F3 N O5

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[3-(4-hydroxyphenyl)-1-oxo-2-propenyl]2,2,4-trimethyl-, (E)- (9CI)

MF C20 H19 N O4

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 2H-1,4-Benzoxazine-7-butanoic acid, 3,4-dihydro-3-oxo- β -phenyl-4-[3-(2-pyridinylamino)propyl]-MF C26 H27 N3 O4

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazin-3(4H)-one, 2,2,4-trimethyl-7-(1-oxo-2-phenyl-2-propen-1-yl)-

MF C20 H19 N O3

$$\begin{array}{c|c} & \text{Me} \\ & & \\ & \text{N} & \text{O} \\ & \text{N} & \text{O} \\ & \text{Me} \\ & \text{H}_2\text{C} & \text{O} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazine-7-butanoic acid,

3,4-dihydro-4-[3-(1H-imidazol-2-ylamino)propyl]-3-oxo- β -phenyl-

MF C24 H26 N4 O4

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & \\ & & \\ &$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxamide, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-N-(2-methoxyethyl)-2,4-dimethyl-3-oxo-, mixt. with 2-[1-(ethoxyimino)butyl]-5-[2-(ethylthio)propyl]-3-hydroxy-2-cyclohexen-1-one (9CI)

CI MXS

$$\begin{array}{c|c} & \text{Me} \\ & \text{N} & \text{O} \\ & \text{N} & \text{O} \\ & \text{Me} \\ & \text{C} - \text{NH} - \text{CH}_2 - \text{CH}_2 - \text{OMe} \\ & \text{O} \end{array}$$

CM 2

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxamide, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-N-[(ethylamino)carbonyl]-3,4-dihydro-2,4-dimethyl-3-oxo
MF C21 H18 C1 F4 N3 O5

$$\begin{array}{c|c} & & & \\ & & &$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazine-2-carboxamide, 7-[2,6-dichloro-4(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-N-2-propen-1-ylMF C21 H17 C12 F3 N2 O4

$$\begin{array}{c|c} & \text{Me} \\ & \text{N} & \text{O} \\ & \text{N} & \text{O} \\ & \text{Me} \\ & \text{C-NH-CH}_2\text{-CH} \\ & \text{CH}_2 \\ & \text{O} \end{array}$$

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxylic acid,

7-[2,6-dichloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-

MF C18 H12 C12 F3 N O5

$$\begin{array}{c|c} & \text{Me} \\ \hline & \text{N} & \text{O} \\ \hline & \text{CO}_2 \text{H} \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazine-3(4H)-thione, 7-[2-chloro-4-(trifluoromethyl)phenoxy]-

2,4-dimethyl-

MF C17 H13 C1 F3 N O2 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 7-(4-chlorobenzoyl)-4-methyl-

MF C16 H12 C1 N O3

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-(4-hydroxyphenyl)acetyl]-4-methyl-MF C17 H15 N O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Methanone, (3,4-dihydro-4-methyl-2H-1,4-benzoxazin-7-y1)(3,5-dimethoxyphenyl)MF C18 H19 N O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2,5-Cyclohexadien-1-one, 4-[[4-(dimethylamino)phenyl](4-ethyl-3,4-dihydro-2H-1,4-benzoxazin-7-yl)methylene]-2,6-dimethoxy
MF C27 H30 N2 O4

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 2-(2-chloroacetyl)-7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-2,4-dimethyl-

MF C19 H13 C12 F4 N O4

$$\begin{array}{c|c} & & & \\ & & &$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

MF C20 H14 C1 F7 N2 O4

CI COM

$$\begin{array}{c|c} & \text{Me} \\ & & \text{N} \\ \hline & \text{O} \\ & \text{Me} \\ \hline & \text{C1} \\ & \text{C} \\ & \text{NH} \\ & \text{CH}_2 \\ & \text{CF}_3 \\ \end{array}$$

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazine-2-carboxylic acid,

7-[2,6-dichloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-, propyl ester

MF C21 H18 C12 F3 N O5

$$\begin{array}{c|c} & & & \\ & & &$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazine-2-carboxylic acid,

7-[2-chloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-4-methyl-3-oxo-, ethylester

MF C19 H15 C1 F3 N O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazin-3(4H)-one, 7-[(2E)-3-(4-hydroxyphenyl)-1-oxo-2-propen-1-yl]-2, 4-dimethyl-

MF C19 H17 N O4

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-(4-hydroxyphenyl)-1-oxo-2-propen-1-yl]2,4-dimethylMF C19 H17 N O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazine-7-butanoic acid,

3, 4-dihydro-3-oxo- β -phenyl-4-[4-(2-pyridinylamino)butyl]-

MF C27 H29 N3 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazin-3(4H)-one, 7-[2,6-dichloro-4-(trifluoromethyl)phenoxy]-2, 4-dimethyl-2-[1-[(2-propyn-1-yloxy)imino]ethyl]-

MF C22 H17 C12 F3 N2 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxamide, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-N-(methylsulfonyl)-3-0xo-

MF C19 H15 C1 F4 N2 O6 S

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazine-2-carboxamide, 7-[2,6-dichloro-4(trifluoromethyl)phenoxy]-N-ethyl-3,4-dihydro-2,4-dimethyl-3-oxoMF C20 H17 C12 F3 N2 O4

$$\begin{array}{c|c} & \text{Me} & \\ & &$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxylic acid,
7-[2-chloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxoMF C18 H13 C1 F3 N O5
CI COM

$$\begin{array}{c|c} & \text{Me} & \\ & &$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-chloro-6-fluoro-4-

(trifluoromethyl)phenoxy]-4-(difluoromethyl)-2-methyl-C17 H10 Cl F6 N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 2H-1,4-Benzoxazin-3(4H)-one, 7-benzoyl-2,2,4-trimethyl-MF C18 H17 N O3

$$\begin{array}{c|c} & Me & \\ & N & O \\ \hline & N & O \\ \hline & Me & \\ O & Me & \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-(4-chlorophenyl)acetyl]-4-methylMF C17 H14 C1 N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2-Propenenitrile, 3-(3,4-dihydro-4-methyl-2H-1,4-benzoxazin-7-yl)-3-(3-ethoxy-4-methoxyphenyl)-

MF C21 H22 N2 O3

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-2,4-dimethylMF C17 H12 C1 F4 N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2,6-dichloro-4-(trifluoromethyl)phenoxy]-2(2-hydroxyacetyl)-2,4-dimethyl
MF C19 H14 C12 F3 N O5

 $\begin{array}{c|c} & \text{Me} & \\ & \text{N} & \text{O} \\ & \text{N} & \text{O} \\ & \text{Me} \\ & \text{C-CH}_2\text{-OH} \end{array}$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazine-2-carboxamide, N-(2-chloroethyl)-7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3, 4-dihydro-2, 4-dimethyl-3-oxo-

MF C20 H16 C12 F4 N2 O4

$$\begin{array}{c|c} & & & \\ & & & \\$$

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

2H-1,4-Benzoxazine-2-carbothioic acid, IN 7-[2-chloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-, S-ethyl ester

C20 H17 C1 F3 N O4 S MF

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):50

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN ΙN 2H-1,4-Benzoxazine, 7-(2,2-diphenylethenyl)-4-ethyl-3,4-dihydro-

MF C24 H23 N O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

REGISTRY COPYRIGHT 2009 ACS on STN L18 246 ANSWERS

IN 2H-1, 4-Benzoxazin-3(4H)-one, 7-[3-(4-hydroxyphenyl)-1-oxo-2-propenyl]-4methyl-, (E)- (9CI)

MF C18 H15 N O4 Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 2H-1,4-Benzoxazine-7-butanoic acid, 3,4-dihydro-4-[(4-methoxyphenyl)methyl]-3-oxo- β -phenyl-, ethyl ester MF C28 H29 N O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-(4-chlorophenyl)-1-oxo-2-propen-1-yl]2,4-dimethylMF C19 H16 C1 N O3

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 4-butyl-8-chloro-7-(4-methoxybenzoyl)-

MF C20 H20 C1 N O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-chloro-6-fluoro-4-

(trifluoromethyl)phenoxy]-2,4-dimethyl-2-(2-methyl-1,3-dioxolan-2-yl)-

MF C21 H18 C1 F4 N O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxamide, 7-[2-chloro-6-fluoro-4-

(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-N-(1-oxopropyl)-

MF C21 H17 C1 F4 N2 O5

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazine-2-carboxamide, 7-[2-chloro-4-(trifluoromethyl)phenoxy]-N-(4,6-dimethyl-2-pyrimidinyl)-3,4-dihydro-2,4-dimethyl-3-oxo-

MF C24 H20 C1 F3 N4 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carbothioic acid,
7-[2-chloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-thioxo, O-ethyl ester

MF C20 H17 C1 F3 N O3 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2,6-dichloro-4-(trifluoromethyl)phenoxy]2,4-dimethyl-

MF C17 H12 C12 F3 N O3

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 2H-1,4-Benzoxazin-3(4H)-one, 7-benzoyl-4-methyl-MF C16 H13 N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 2H-1,4-Benzoxazin-3(4H)-one, 4-methyl-7-(2-phenylacetyl)-MF C17 H15 N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2-Propenenitrile, 3-(3,4-dihydro-4-methyl-2H-1,4-benzoxazin-7-yl)-3-(3,5-dimethoxyphenyl)-

MF C20 H20 N2 O3

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN β -Alanine, N-[[7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-2H-1,4-benzoxazin-2-yl]carbonyl]-, ethyl ester, mixt. with ethyl 2-[4-[(6-chloro-2-benzoxazolyl)oxy]phenoxy]propanoate (9CI)

MF C23 H21 C1 F4 N2 O6 . C18 H16 C1 N O5

CI MXS

CM 1

CM 2

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-2-(2-hydroxyacetyl)-2,4-dimethyl-

MF C19 H14 C1 F4 N O5

$$\begin{array}{c|c} & & \text{Me} \\ & & \text{N} \\ & & \text{O} \\ & & \text{Me} \\ & & \text{O} \\ & & \text{C-CH}_2\text{-OH} \\ & & \text{O} \\ \end{array}$$

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IN 2H-1,4-Benzoxazine-2-carboxamide, 7-[2-chloro-6-fluoro-4(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-N-2-propyn-1-yl
MF C21 H15 C1 F4 N2 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxylic acid,
7-[2-chloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-,
2-methoxyethyl ester

MF C21 H19 C1 F3 N O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[3-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-oxo-2-propen-1-yl]-4-methyl-

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2H-1, 4-Benzoxazin-3(4H)-one, 7-[3-(4-chlorophenyl)-1-oxo-2-propenyl]-2, 2, 4-IN trimethyl-, (E)- (9CI) C20 H18 Cl N O3

MF

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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INDEX NAME NOT YET ASSIGNED ΙN

MFC33 H41 N3 O6

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IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-(4-hydroxyphenyl)-1-oxo-2-propen-1-yl]-4methyl-

MF C18 H15 N O4

$$\begin{array}{c|c} & \text{Me} \\ & \\ & \\ \text{C} \\ \text{C} \\ \text{CH}_2 \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN Methanone, [4-[2-(3,4-dimethoxyphenyl)ethyl]-3,4-dihydro-2H-1,4-benzoxazin-7-yl][3-methoxy-4-(methylamino)phenyl]-

MF C27 H30 N2 O5

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-2,4-dimethyl-2-[1-(2-methylhydrazinylidene)ethyl]MF C20 H18 C1 F4 N3 O3

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN 2H-1,4-Benzoxazine-2-carboxamide, N-acetyl-7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo
MF C20 H15 C1 F4 N2 O5

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazine-2-carboxamide, 7-[2-chloro-4-(trifluoromethyl)phenoxy]-

N, N-diethyl-3, 4-dihydro-2, 4-dimethyl-3-oxo-MF C22 H22 Cl F3 N2 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN 2H-1,4-Benzoxazine-2-carboxylic acid,
7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-4-(difluoromethyl)-3,4dihydro-2-methyl-3-oxo-, ethyl ester

MF C20 H14 C1 F6 N O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 2H-1,4-Benzoxazin-3(4H)-one, 2,4-dimethyl-7-phenoxy-MF C16 H15 N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1, 4-Benzoxazine-4-carboxamide, 6-bromo-7-(4-bromophenoxy)-2, 3-dihydro-N-methyl-

MF C16 H14 Br2 N2 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,2-Ethanedione, 1-(3,4-dihydro-4-methyl-2H-1,4-benzoxazin-7-yl)-2-phenyl-MF C17 H15 N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazin-3(4H)-one, 4-methyl-7-(phenyl-1H-1, 2, 4-triazol-1-ylmethyl)-

MF C18 H16 N4 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN β -Alanine, N-[[7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-2H-1,4-benzoxazin-2-yl]carbonyl]-, ethyl ester, mixt. with ethyl 2-[4-[(6-chloro-2-quinoxalinyl)oxy]phenoxy]propanoate (9CI)

MF C23 H21 C1 F4 N2 O6 . C19 H17 C1 N2 O4

CI MXS

CM 1

CM 2

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 2-acetyl-7-[2,6-dichloro-4-(trifluoromethyl)phenoxy]-2,4-dimethyl-

MF C19 H14 C12 F3 N O4

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxamide, 7-[2-chloro-6-fluoro-4(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-N-2-propen-1-yl
MF C21 H17 C1 F4 N2 O4

$$\begin{array}{c|c}
 & \text{Me} \\
\hline
 & \text{N} \\
\hline
 & \text{O} \\
\hline
 & \text{Me} \\
\hline
 & \text{O} \\
\hline
 & \text{C-NH-CH}_2\text{-CH} \\
\hline
 & \text{CH}_2
\end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxylic acid,
7-[2-chloro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-3-oxo-,
2-oxopropyl ester

MF C21 H17 C1 F3 N O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[3-fluoro-5-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenoxy]-4-methyl-

MF C21 H22 F N O5

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[(2E)-3-(4-chlorophenyl)-1-oxo-2-propen-1-yl]-2,4-dimethyl
MF C19 H16 C1 N O3

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN INDEX NAME NOT YET ASSIGNED MF C23 H27 N5 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazin-3(4H)-one, 7-[2-(4-chlorophenyl)-1-oxo-2-propen-1-yl]-4-methyl-

MF C18 H14 C1 N O3

$$\begin{array}{c|c} & \text{Me} \\ & \\ & \\ \text{C} \\ & \\ \text{CH}_2 \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Methanone, [4-[2-(3,4-dimethoxyphenyl)ethyl]-3,4-dihydro-2H-1,4-benzoxazin-7-yl][4-[[2-(3,4-dimethoxyphenyl)ethyl]methylamino]phenyl]-

MF C36 H40 N2 O6

$$\begin{array}{c} \text{OMe} \\ \text{MeO} \\ \text{OMe} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{N} \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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MF C24 H23 C12 F3 N2 O6

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxamide, 7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-N-[2-(ethylamino)-1-methyl-2-oxoethyl]-3,4-dihydro-2,4-dimethyl-3-oxo-

MF C23 H22 C1 F4 N3 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1, 4-Benzoxazine-2-carboxamide, 7-[2-chloro-4-(trifluoromethyl)phenoxy]-3, <math>4-dihydro-N-methoxy-N, 2, 4-trimethyl-3-oxo-

MF C20 H18 C1 F3 N2 O5

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazine-2-carboxylic acid,

7-[2-chloro-6-fluoro-4-(trifluoromethyl)phenoxy]-3,4-dihydro-2,4-dimethyl-

3-oxo-, ethyl ester

MF C20 H16 C1 F4 N O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1,4-Benzoxazin-3(4H)-one, 7-[2-chloro-4-(trifluoromethyl)phenoxy]-4-

(hydroxymethyl)-2-methyl-

MF C17 H13 C1 F3 N O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L18 246 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 4H-1,4-Benzoxazine-4-carboxamide, 2,3-dihydro-N-methyl-7-phenoxy-

MF C16 H16 N2 O3

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